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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 08	X.25 communication option no longer available after June 2006
NEWS 10	MAR 22	EMBASE is now updated on a daily basis
NEWS 11	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 12	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 13	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 14	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 15	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 16	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 17	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 18	MAY 11	KOREAPAT updates resume

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* *

COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

Dear valued STN customer,

In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW

Thank you in advance for your participation.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:54:15 ON 16 MAY 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:54:24 ON 16 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 MAY 2006 HIGHEST RN 884382-45-0
DICTIONARY FILE UPDATES: 15 MAY 2006 HIGHEST RN 884382-45-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

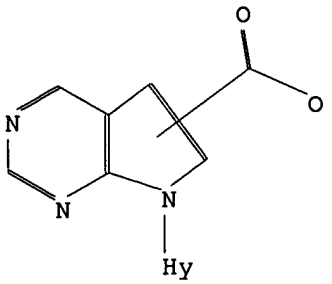
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

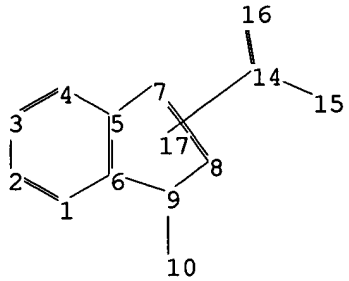
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10500040f.str





chain nodes :
10 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
9-10 14-16 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 9-10 14-16 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:Hy,Cb,Cy

G2:Cl,O

G3:CO2H,C(O)CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> s l1 full
FULL SEARCH INITIATED 15:54:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 52422 TO ITERATE

100.0% PROCESSED 52422 ITERATIONS 52 ANSWERS
SEARCH TIME: 00.00.02

L2 52 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'CAPLUS' ENTERED AT 15:54:47 ON 16 MAY 2006
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FILE COVERS 1907 - 16 May 2006 VOL 144 ISS 21
FILE LAST UPDATED: 15 May 2006 (20060515/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2

L3 65 L2

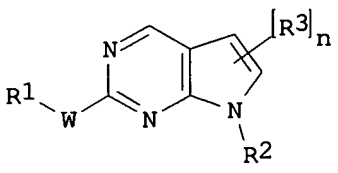
=> d l3 ibib abs hitstr

L3 ANSWER 1 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1220346 CAPLUS
DOCUMENT NUMBER: 143:477978
TITLE: Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation
INVENTOR(S): Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter
PATENT ASSIGNEE(S): IRM LLC, Bermuda
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005107760	A1	20051117	WO 2005-US15118	20050429

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-567346P P 20040430
OTHER SOURCE(S): MARPAT 143:477978
GI



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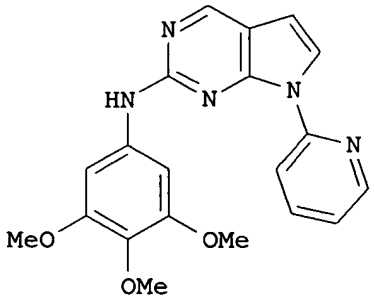
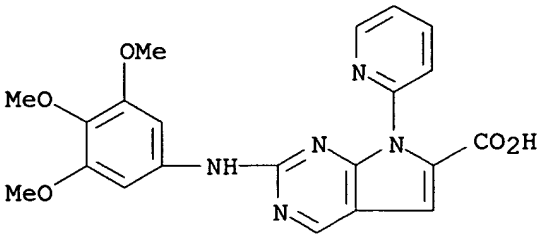


II

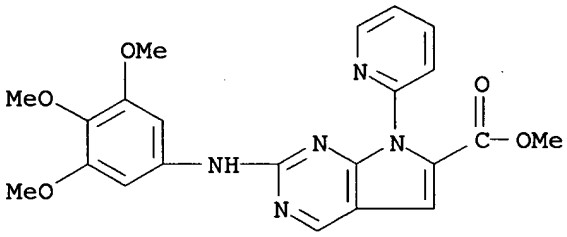
AB The invention provides compds. I [n = 0-2; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R2 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

IT **863597-79-9P 863597-80-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of

keratinocyte differentiation)
RN 863597-79-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 863597-80-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l3 ibib abs hitstr 1-65

L3 ANSWER 1 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1220346 CAPLUS
DOCUMENT NUMBER: 143:477978
TITLE: Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation
INVENTOR(S): Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter
PATENT ASSIGNEE(S): IRM LLC, Bermuda
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
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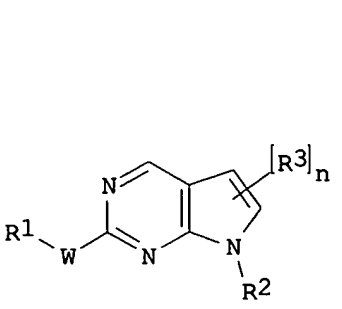
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2004-567346P P 20040430
OTHER SOURCE(S): MARPAT 143:477978

GI



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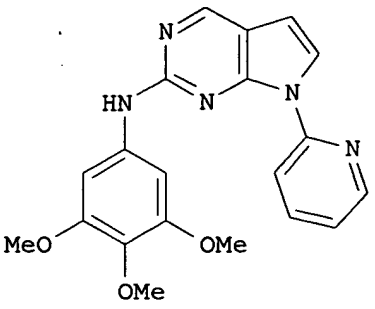


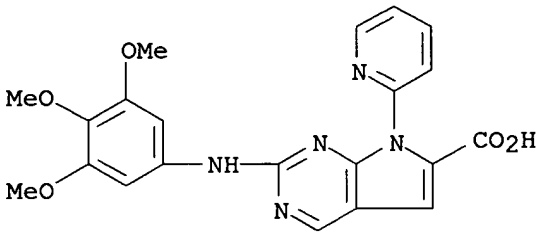
II

AB The invention provides compds. I [n = 0-2; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R2 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

IT **863597-79-9P 863597-80-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation)

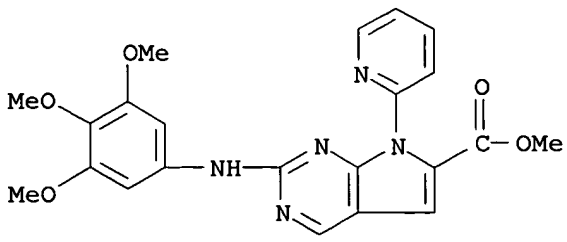
RN 863597-79-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 863597-80-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:962258 CAPLUS
DOCUMENT NUMBER: 143:266947
TITLE: Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors
INVENTOR(S): Choi, Ha-Soon; Wang, Zhicheng; Gray, Nathanael Schiander; Gu, Xiang-Ju; He, Xiaohui; He, Yun; Jiang, Tao; Liu, Yi; Richmond, Wendy; Sim, Taebo; Yang, Kunyong
PATENT ASSIGNEE(S): IRM LLC, Bermuda
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080393	A1	20050901	WO 2005-US4630	20050214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

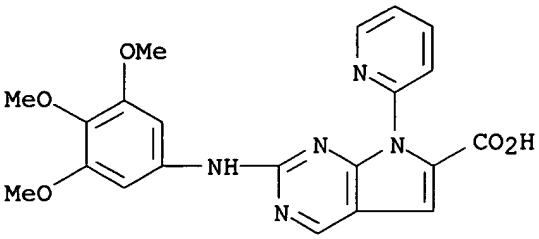
PRIORITY APPLN. INFO.: US 2004-544944P P 20040214
OTHER SOURCE(S): MARPAT 143:266947
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

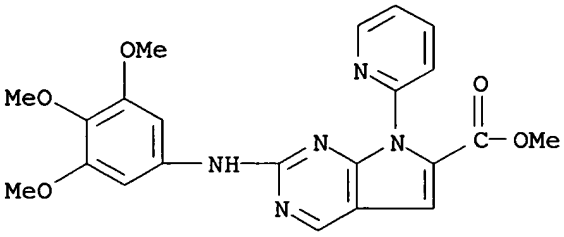
AB The invention provides a novel class of compds. I-V [n = 0-2; m = 0-3; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = (un)substituted (hetero)arylakyl, (hetero)cycloalkyl; R2 = (un)substituted (hetero)arylakyl, (hetero)cycloalkyl; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with abnormal or deregulated kinase activity, particularly diseases or disorders that involve abnormal activation of the FAK, Abl, BCR-Abl, PDGF-R, c-Kit, NPM-ALK, Flt-3, JAK2 and c-Met kinases. Over 200 compds. I-V were prepared and characterized. The preparation of the compds. I is illustrated in examples. E.g., synthesis of I [R1 = 3,4,6-(MeO)3C6H2; R2 = 2-pyridyl; R3 = H; W = NH], starting from 5-bromo-2,4-dichloropyrimidine, was given. The compds. I-V were tested against various kinases. For example, they inhibit the enzyme activity by 50% (IC50), in a concentration of from 0.001 to 0.5 μM, especially from 0.01 to 0.1 μM.

IT **863597-79-9P 863597-80-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn of pyrrolopyrimidines and their analogs as protein kinase inhibitors)

RN 863597-79-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



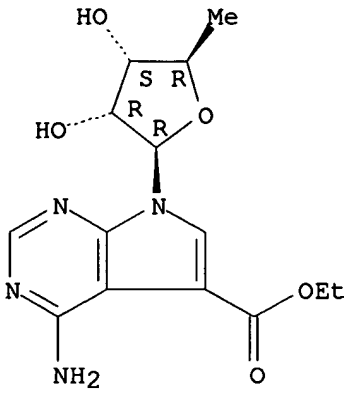
RN 863597-80-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-pyridinyl)-2-[(3,4,5-trimethoxyphenyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:372245 CAPLUS
DOCUMENT NUMBER: 143:125813
TITLE: QSAR studies on adenosine kinase inhibitors
AUTHOR(S): Agrawal, Vijay K.; Singh, Kamana; Khadikar, Padmakar V.
CORPORATE SOURCE: QSAR and Computer Chemical Laboratories, A.P.S. University, Rewa, 486 003, India
SOURCE: Medicinal Chemistry Research (2004), 13(6/7), 479-496
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The present study reports QSAR study on adenosine kinase inhibitors pyrrolo[2,3-d] pyrimidine nucleoside analogs. The equalized electronegativity along with a large pool of topol. indexes are used for the purpose. The regression anal. has shown that equalized electronegativity is a good parameter which in combination with topol. indexes and an indicator parameter gave excellent model.
IT **144928-02-9**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(QSAR studies on adenosine kinase inhibitors)
RN 144928-02-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:216597 CAPLUS
DOCUMENT NUMBER: 142:291323
TITLE: Compositions and methods for the treatment of severe acute respiratory syndrome (SARS)
INVENTOR(S): Hardee, Greg; Dellamary, Luis
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 217 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020885	A2	20050310	WO 2004-US16196	20040521
WO 2005020885	A3	20050804		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

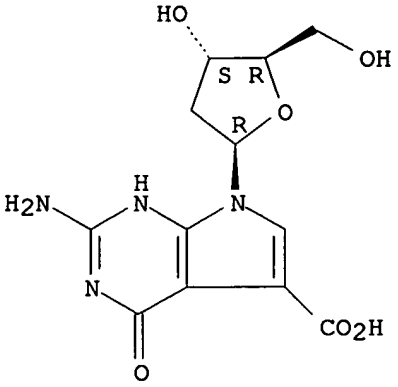
PRIORITY APPLN. INFO.: US 2003-472774P P 20030521

AB The invention provides compns. and methods for treating a coronavirus infection, especially a SARS CoV infection. The compns. comprise an antiviral nucleoside or mimetic thereof, or an antiviral antisense agent, in a form suitable for pulmonary or nasal delivery. The methods comprise administration to a patient in need thereof the effective amount of an antiviral composition by pulmonary or nasal instillation.

IT **124738-85-8 443642-56-6**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. and methods for treatment of severe acute respiratory syndrome)

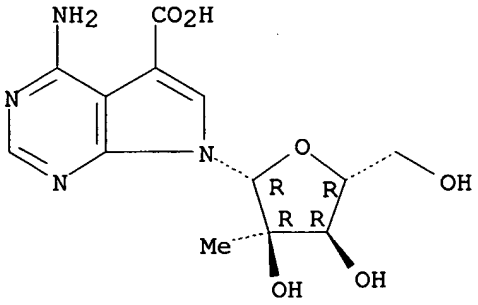
RN 124738-85-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443642-56-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 5 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:199486 CAPLUS
DOCUMENT NUMBER: 142:441277
TITLE: QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices
AUTHOR(S): Gonzalez-Diaz, Humberto; Cruz-Monteagudo, Maykel; Vina, Dolores; Santana, Lourdes; Uriarte, Eugenio; De Clercq, Erik
CORPORATE SOURCE: Department of Organic Chemistry, Faculty of Pharmacy, University of Santiago de Compostela, 15782, Spain
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(6), 1651-1657
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

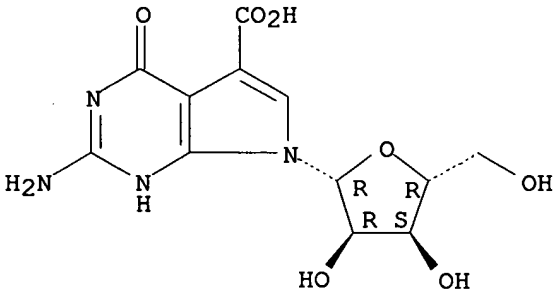
AB The unified representation of spectral moments, classic topol. indexes, quadratic indexes, and stochastic mol. descriptors show that all these mol. descriptors lie within the same family. Consequently, the same prior probability for a successful quant. structure-activity relation (QSAR) may be expected irresp. of which indexes are selected. Herein, we used stochastic spectral moments as mol. descriptors to seek a QSAR using a database of 221 bioactive compds. previously tested against diverse RNA viruses and 402 nonactive ones. The QSAR model thus obtained correctly classifies 90.9% of compds. in training. The model also correctly classifies a total of 87.9% of 207 compds. on addnl. external predicting series, 73 of them having anti-RNA-virus activity and 134 nonactive ones. In addition, all compds. were regrouped into five different subsets for leave-group-out studies: (1) anti-influenza, (2) anti-picornavirus, (3) anti-paramyxovirus, (4) anti-RSV/anti-influenza, and (5) broad range

anti-RNA-virus activity. The model has retained overall accuracies of about 90% on these studies validating model robustness. Finally, we exemplify the practical use of the model with the discovery of compds. 124 and 128. These compds. presented MIC50 values = 3.2 and 8 μg/mL against respiratory syncytial virus (RSV) resp. Both compds. also have low cytotoxicity expressed by their Minimal Cytotoxic Concns. >400 μg/mL for HeLa cells. The present approach represents an effort toward a formalization and application of mol. indexes in bioorg. and medicinal chemical

IT **81645-08-1 851071-69-7 851071-70-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides)

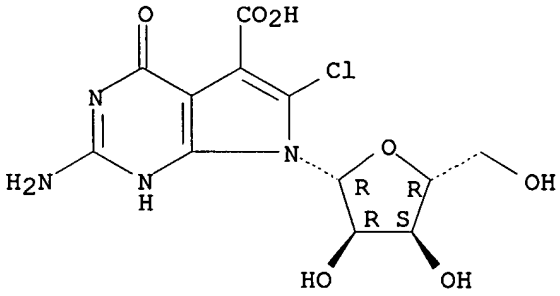
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



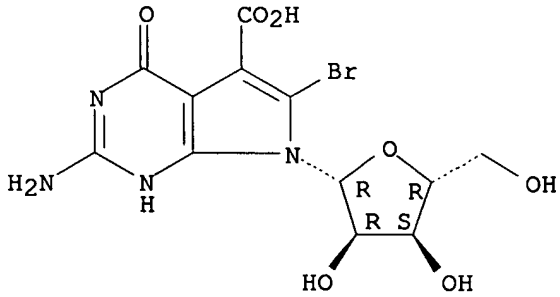
RN 851071-69-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-6-chloro-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 851071-70-0 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-6-bromo-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:773084 CAPLUS

DOCUMENT NUMBER: 141:388156

TITLE: Structure-Activity Relationship of Heterobase-Modified 2'-C-Methyl Ribonucleosides as Inhibitors of Hepatitis C Virus RNA Replication

AUTHOR(S): Eldrup, Anne B.; Prhavc, Marija; Brooks, Jennifer; Bhat, Balkrishen; Prakash, Thazha P.; Song, Quanlai; Bera, Sanjib; Bhat, Neelima; Dande, Prasad; Cook, P. Dan; Bennett, C. Frank; Carroll, Steven S.; Ball, Richard G.; Bosserman, Michele; Burlein, Christine; Colwell, Lawrence F.; Fay, John F.; Flores, Osvaldo A.; Getty, Krista; LaFemina, Robert L.; Leone, Joseph; MacCoss, Malcolm; McMasters, Daniel R.; Tomassini, Joanne E.; Von Langen, Derek; Wolanski, Bohdan; Olsen, David B.

CORPORATE SOURCE: Department of Medicinal Chemistry, Isis Pharmaceuticals, Carlsbad, CA, 92008, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(21), 5284-5297
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:388156

AB Hepatitis C virus infection constitutes a significant health problem in need of more effective therapies. The authors have recently identified 2'-C-methyladenosine and 2'-C-methylguanosine as potent nucleoside inhibitors of HCV RNA replication in vitro. However, both of these compds. suffered from significant limitations. 2'-C-Methyladenosine was found to be susceptible to enzymic conversions by adenosine deaminase and purine nucleoside phosphorylase, and it displayed limited oral bioavailability in the rat. 2'-C-Methylguanosine, on the other hand, was neither efficiently taken up in cells nor phosphorylated well. As part of an attempt to address these limitations, the authors now report upon the synthesis and evaluation of a series of heterobase-modified 2'-C-Me ribonucleosides. The structure-activity relationship within this series of nucleosides reveals 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine and 4-amino-5-fluoro-7-(2-C-methyl-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine as potent and noncytotoxic inhibitors of HCV RNA replication. Both 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine and 4-amino-5-fluoro-7-(2-C-methyl-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine display improved enzymic stability profiles as compared to that of 2'-C-methyladenosine. Consistent with these observations, the most potent compound, 4-amino-5-fluoro-7H-pyrrolo[2,3-d]pyrimidine ribonucleoside, is orally bioavailable in the rat. Together, the potency of the 2'-C-methyl-4-amino-pyrrolo[2,3-d]pyrimidine ribonucleosides and their improved pharmacokinetic properties relative to that of 2'-C-methyladenosine suggests that this class of compds. may have clin. utility.

IT **443642-56-6P**

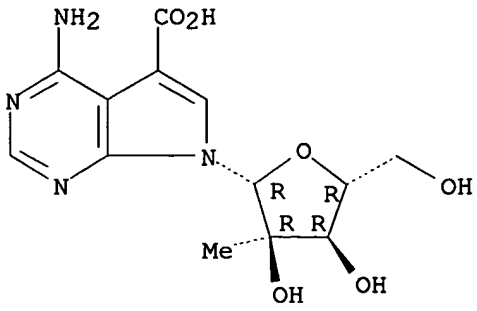
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structure-activity relationship of heterobase-modified 2'-C-Me ribonucleosides as inhibitors of hepatitis C virus RNA replication)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

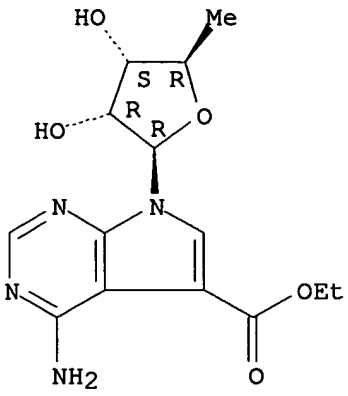
L3 ANSWER 7 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:403777 CAPLUS
DOCUMENT NUMBER: 141:169851
TITLE: A TOPS-MODE approach to predict adenosine kinase inhibition
AUTHOR(S): Gonzalez, Maykel Perez; Moldes, Maria del Carmen Teran
CORPORATE SOURCE: Service Unit, Experimental Sugar Cane Station 'Villa Clara-Cienfuegos', Villa Clara, C.P. 53100, Cuba
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(12), 3077-3079
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The TOPol. Sub-Structural Mol. Design (TOPS-MODE) approach has been used to address the adenosine kinase inhibitory activity of pyrrolo[2,3-d]pyrimidine nucleoside analogs. A model capable of describing around 77% of the variance in exptl. activity of 32 analogs was developed on the basis of this approach. In contrast, out of nine different approaches, including the use of Constitutional, Topol., BCUT, 2D autocorrelations, geometrical, RDF, 3D Morse, WHIM, and GETAWAY descriptors none were able to explain more than 70% of the variance in the above-mentioned property with the same number of descriptors. Although statistically significant models were derived containing descriptors other than spectral moments, the model that exhibited the best fit was based on these variables.

IT **144928-02-9**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(TOPS-MODE approach permits QSAR anal. of adenosine kinase inhibition by pyrrolo[2,3-d]pyrimidine nucleoside analogs)

RN 144928-02-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:951160 CAPLUS
DOCUMENT NUMBER: 140:13688
TITLE: Oligonucleotides having modified nucleoside units with various linkages, and their uses as antisense agents, ribozymes, aptamers, siRNA, probes, and primers, or when hybridized to RNA, as substrates for RNA cleaving enzymes
INVENTOR(S): Eldrup, Anne; Cook, Phillip Dan; Parshall, Lynne B.
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 161 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003100017	A2	20031204	WO 2003-US16526		20030523
WO 2003100017	A3	20040826			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2003241621	A1	20031212	AU 2003-241621		20030523
US 2004014108	A1	20040122	US 2003-444298		20030523
PRIORITY APPLN. INFO.:			US 2002-383358P	P	20020524
			WO 2003-US16526	W	20030523

OTHER SOURCE(S): MARPAT 140:13688

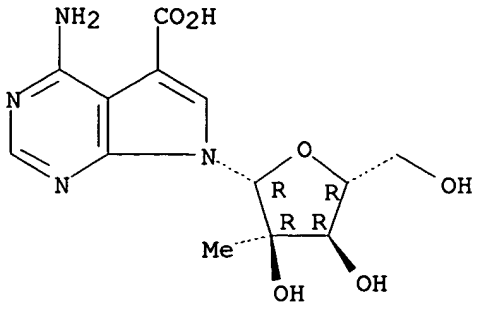
AB Disclosed are oligonucleotides that include one or more modified nucleoside units. The examples present the representative preparation of modified nucleosides and nucleoside amidites, for incorporation into said oligonucleotides. The oligonucleotides are particularly useful as antisense agents, ribozymes aptamer, siRNA agents, probes and primers or, when hybridized to an RNA, as a substrate for RNA cleaving enzymes including Rnase H and dsRNase.

IT **443642-56-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of modified nucleosides and nucleoside amidites for incorporation into oligonucleotides, and uses)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 9 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:951042 CAPLUS
DOCUMENT NUMBER: 140:24085
TITLE: Oligonucleotides having modified nucleoside units with various linkages, and their uses as antisense agents, ribozymes, aptamers, siRNA, probes, and primers, or when hybridized to RNA, as substrates for RNA cleaving enzymes
INVENTOR(S): Eldrup, Anne; Cook, Phillip Dan; Parshall, B. Lynne
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 271 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003099840	A1	20031204	WO 2003-US16502		20030523
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2003237249	A1	20031212	AU 2003-237249		20030523
US 2004014957	A1	20040122	US 2003-444628		20030523
PRIORITY APPLN. INFO.:			US 2002-383438P	P	20020524
			WO 2003-US16502	W	20030523

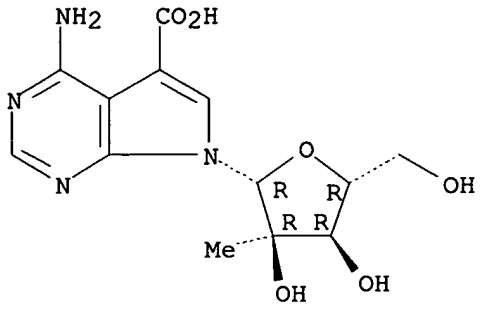
OTHER SOURCE(S): MARPAT 140:24085

AB Disclosed are oligonucleotides that include one or more modified nucleoside units. The examples present the representative preparation of modified nucleosides and nucleoside amidites, for incorporation into said oligonucleotides. The oligonucleotides are particularly useful as antisense agents, ribozymes aptamer, siRNA agents, probes and primers or, when hybridized to an RNA, as a substrate for RNA cleaving enzymes including Rnase H and dsRNase.

IT **443642-56-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(oligonucleotides having modified nucleoside units with various linkages)

RN 443642-56-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

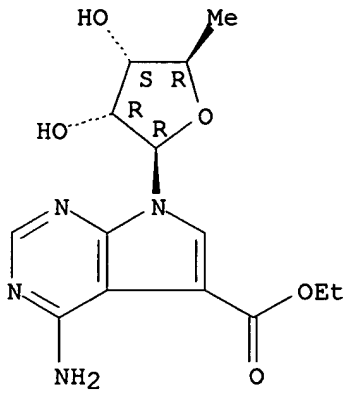
L3 ANSWER 10 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:681321 CAPLUS
DOCUMENT NUMBER: 140:246064
TITLE: Quantitative Structure-Activity Relationship Study of 5-Iodo- and Diaryl-analogues of Tubercidin: Inhibitors of Adenosine Kinase
AUTHOR(S): Singh, P.; Kumar, Rajesh; Sharma, B. K.
CORPORATE SOURCE: Dep. Chem., S.K. Government Coll., Sikar, 332 001, India
SOURCE: Journal of Enzyme Inhibition and Medicinal Chemistry (2003), 18(5), 395-402
CODEN: JEIMAZ; ISSN: 1475-6366
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The adenosine kinase inhibitory (AKI) activity of 5-iodo and diaryl analogs of tubercidin is quant. analyzed using Fujita-Ban and Hansch type analyses. The Fujita-Ban anal. being a non-parametric approach assigned the highest contribution to Cl at the X-position, C6H4-4-Cl, C6H5, 2-furanyl and I at the Y-position and CH2NH2 and CH3 at the Z-position. In addition, a OH substituent at the C-position also emerged as a better choice possibly due to its engagement in hydrogen bonding with some active site function. Thus a compound having Cl, C6H4-4-Cl, CH2NH2 and OH resp. at X-, Y-, Z- and C-positions is predicted to have a potency nearly 1.5 orders of magnitude higher than the most potent compound of the parent data set. The Hansch type anal., on the other hand, is a parametric approach and is carried out on two sub-sets of original compds. This sub-division is based on size and nature of the substituents present at the X- and Y-positions. For the compds. in the first sub-set the derived significant correlation equation suggested that the substituent at the Y-position exhibiting a higher field effect and a substituent such as Cl and CH2NH2 at X- and Z-positions, resp., are important for a compound to show increased AKI activity. Thio/alkylthio at X and CH2OCH3 at Z, on the other hand, lead to a detrimental effect. Similarly for the compds. in the second sub-set, the derived significant correlation equation showed that a substituent at the X-position having a higher neg. field effect, a substituent at the Y-position having bulky groups and the C-position occupied by a OH group are essential for enhancement of the activity of a compound

IT **144928-02-9**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(quant. structure-activity relationship study of 5-iodo- and diaryl-analogs of tubercidin as inhibitors of adenosine kinase)

RN 144928-02-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:656596 CAPLUS
DOCUMENT NUMBER: 139:191380
TITLE: Methods of inhibiting orthopoxvirus replication with nucleoside compounds
INVENTOR(S): Olsen, David B.; Lafemina, Robert L.; Eldrup, Anne B.; Bera, Sanjib
PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003068244	A1	20030821	WO 2003-US3703	20030207
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2474563	AA	20030821	CA 2003-2474563	20030207
AU 2003209045	A1	20030904	AU 2003-209045	20030207
EP 1476169	A1	20041117	EP 2003-707772	20030207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005164960	A1	20050728	US 2003-504445	20030207
JP 2005527499	T2	20050915	JP 2003-567425	20030207

PRIORITY APPLN. INFO.: US 2002-356805P P 20020213
WO 2003-US3703 W 20030207

OTHER SOURCE(S): MARPAT 139:191380

AB The present invention provides methods of inhibiting orthopoxvirus replication and/or treating orthopoxvirus infection with certain nucleoside compds. and derivs. thereof. These compds. are particularly useful as inhibitors of vaccinia virus and variola virus replication and/or for the treatment of vaccinia virus and variola virus infection. The nucleoside compds. may be administered alone or in combination with other agents active against orthopoxvirus infection, in particular against vaccinia virus or variola virus infection. Another aspect of the present invention provides for the use of such nucleoside compds. in the manufacture of a medicament for the inhibition of orthopoxvirus replication and/or for

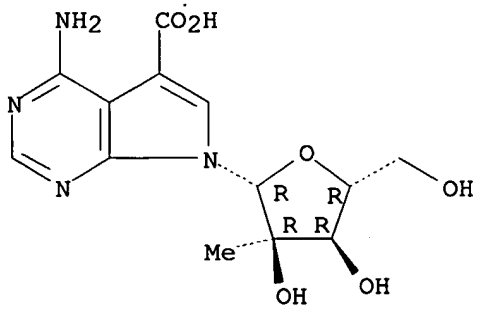
the treatment of orthopoxvirus infection. Yet a further aspect of the present invention provides such nucleoside compds. for use as a medicament for the inhibition of orthopoxvirus replication and/or for the treatment of orthopoxvirus infection.

IT **443642-56-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibiting orthopoxvirus replication with nucleoside compds.)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

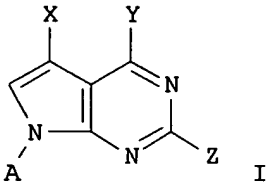
L3 ANSWER 12 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:590940 CAPLUS
DOCUMENT NUMBER: 139:133787
TITLE: Preparation of deazapurine nucleoside analogs as antiviral agents
INVENTOR(S): An, Haoyun; Ding, Yili; Chamakura, Varaprasad; Hong, Zhi
PATENT ASSIGNEE(S): Ribapharm Inc., USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003061576	A2	20030731	WO 2003-US1545	20030117
WO 2003061576	A3	20040401		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-350296P P 20020117
OTHER SOURCE(S): MARPAT 139:133787
GI



I

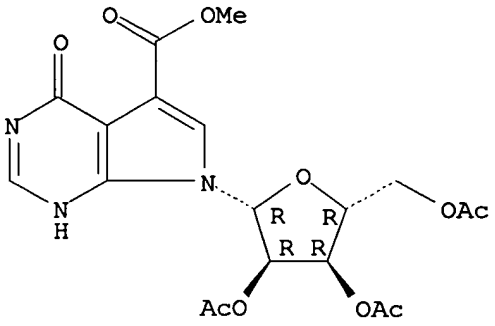
AB Methods, compns., and uses for various deazapurine nucleoside libraries and library compds. I are provided. Particularly preferred deazapurine nucleosides include 7-deazapurine nucleosides, 7-deaza-8-azapurine nucleosides, toyocamycin nucleoside analogs, 3-deazapurine nucleosides, and 9-deazapurine nucleosides, while preferred uses especially include use of such compds. as pharmacol., and particularly antiviral agents. 4-N,N-dimethylamino-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine-5-N-hydroxycarbamidine was prepared and tested in vitro as antiviral agent.

IT **565455-12-1P 565455-13-2P 565455-22-3P**
565455-23-4DP, resin bound **565455-23-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deazapurine nucleoside analogs as antiviral agents)

RN 565455-12-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

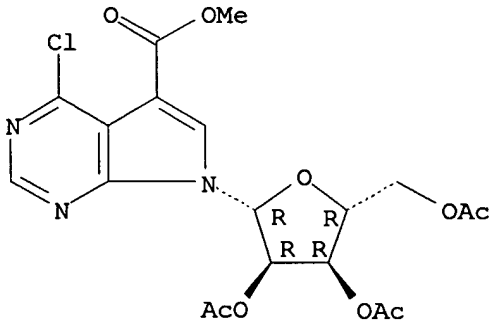
Absolute stereochemistry.



RN 565455-13-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

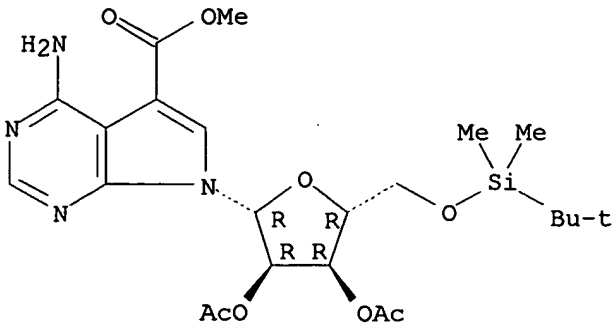
Absolute stereochemistry.



RN 565455-22-3 CAPLUS

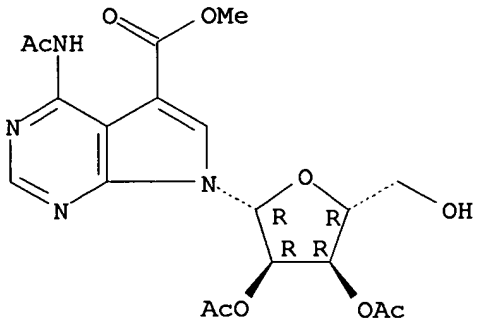
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



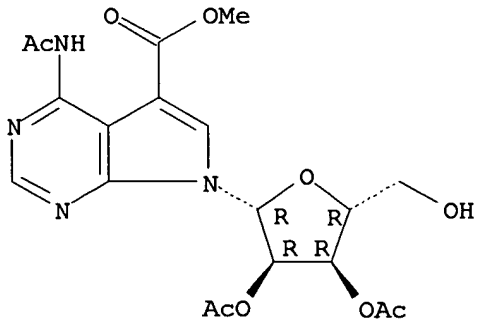
RN 565455-23-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-β-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 565455-23-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-β-D-ribofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 13 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:506580 CAPLUS
DOCUMENT NUMBER: 139:79178
TITLE: Synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivatives and use as phosphodiesterase VII inhibitors and in combination with other agents
INVENTOR(S): Eggenweiler, Hans-Michael; Wolf, Michael
PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10163991	A1	20030703	DE 2001-10163991	20011224
CA 2471538	AA	20030710	CA 2002-2471538	20021108
WO 2003055882	A1	20030710	WO 2002-EP12533	20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002367090	A1	20030715	AU 2002-367090	20021108
EP 1458722	A1	20040922	EP 2002-805744	20021108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002015308	A	20041221	BR 2002-15308	20021108
CN 1608067	A	20050420	CN 2002-826034	20021108
JP 2005520801	T2	20050714	JP 2003-556412	20021108
US 2005059686	A1	20050317	US 2004-500040	20040623
ZA 2004005859	A	20050517	ZA 2004-5859	20040722
PRIORITY APPLN. INFO.:			DE 2001-10163991 A	20011224
			WO 2002-EP12533 W	20021108

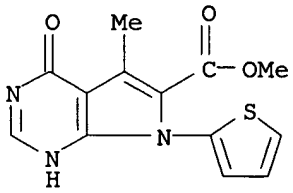
OTHER SOURCE(S): MARPAT 139:79178

AB The invention concerns the synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs., their physiol. acceptable salts, stereoisomers, solvates, mixts. thereof and their use as phosphodiesterase VII inhibitors in the treatment of diseases that are influenced by the phosphodiesterase VII regulation of human eosinophil activation and degranulation. Osteoporesis, tumors, cachexia, atherosclerosis, rheumatoid arthritis, multiple sclerosis, diabetes mellitus, AIDS, autoimmune and heart diseases can be treated with the drugs. Thus the synthesis of 5-isopropyl-4-oxo-7-p-tolyl-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid Et ester and analog compds. is described along with injection, suppository, tablet and other formulations.

IT **552298-62-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs. and use as phosphodiesterase VII inhibitors and in combination with other agents)

RN 552298-62-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-(2-thienyl)-, methyl ester (9CI) (CA INDEX NAME)



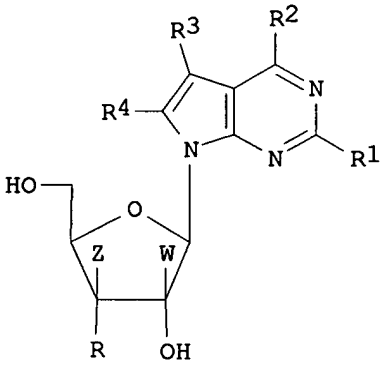
L3 ANSWER 14 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2003:491245 CAPLUS
DOCUMENT NUMBER:	139:53258
TITLE:	Solid phase synthesis and combinatorial libraries of deazapurine nucleosides useful in the treatment of viral infections and neoplastic diseases
INVENTOR(S):	Girardet, Jean-Luc; An, Haoyun; Chamakura, Varaprasad; Gunic, Esmir; Hong, Zhi
PATENT ASSIGNEE(S):	Ribapharm Inc., USA

SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003051899	A1	20030626	WO 2002-US40416		20021217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2002353165	A1	20030630	AU 2002-353165		20021217
PRIORITY APPLN. INFO.:			US 2001-342410P	P	20011217
			WO 2002-US40416	W	20021217

OTHER SOURCE(S): MARPAT 139:53258
GI



I

AB Deazapurine nucleoside analogs I, wherein R is H, OH; R1-R4 are independently H, halogen, NH2, NHR', R', CN, CONH2, N3, CH2CN; R' is substituted alkyl, unsubstituted alkyl, substituted aryl, and an unsubstituted aryl; W and Z are independently hydrogen, N3, NH2, OH, SH, R5, or NHR5 wherein R5 is an alkyl, substituted alkyl, alkenyl, a substituted alkenyl, alkynyl, substituted alkynyl, aryl, substituted aryl; are prepared in a combinatorial library approach. Particularly preferred compds. and libraries include various 7-deazapurines, 9-deazapurines, and 7-deaza-8-azaguanosine as heterocyclic bases, and it is generally preferred that such nucleosides include a ribofuranose as the sugar moiety. It is further contemplated that compds. generated using contemplated libraries may be useful in the treatment of various conditions, particularly viral infections and neoplastic diseases (no data). Thus, I (R = OH; R1 = R4 = Z = W = H; R2 = NHBn; R3 = Ph) was prepared useful in the treatment of viral infections and neoplastic diseases.

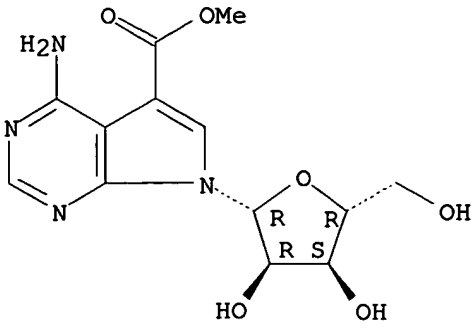
IT **18440-68-1P 547754-20-1P 547754-21-2P 547754-22-3P 547754-23-4DP**, 4-methoxytrityl resin support **547754-23-4P 547754-24-5DP**, 4-methoxytrityl resin support **547754-37-0P 547754-38-1DP**, 4-methoxytrityl resin support **547754-38-1P 547754-39-2DP**, 4-methoxytrityl resin support
RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(solid phase synthesis and combinatorial libraries of deazapurine nucleosides useful in treatment of viral infections and neoplastic diseases)

RN 18440-68-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

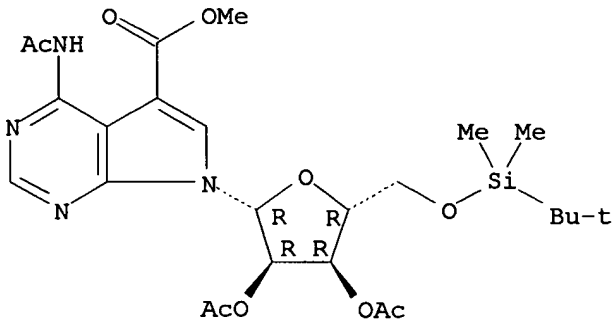
Absolute stereochemistry.



RN 547754-20-1 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

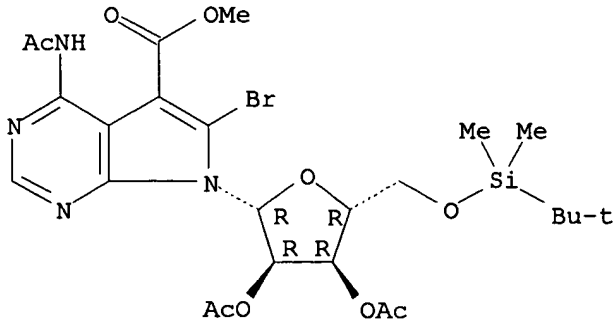
Absolute stereochemistry.



RN 547754-21-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-6-bromo-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

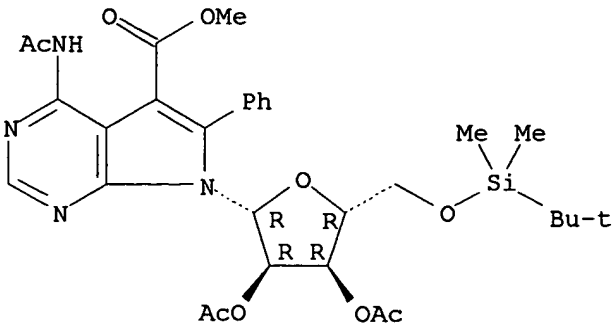
Absolute stereochemistry.



RN 547754-22-3 CAPLUS

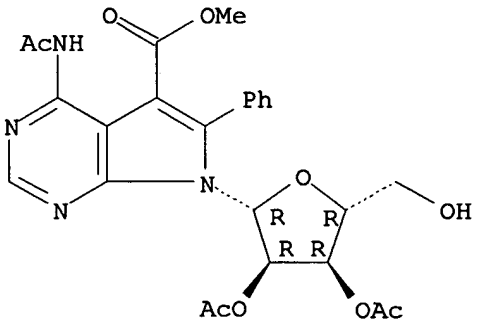
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-[2,3-di-O-acetyl-5-O-[(1,1-dimethylethyl)dimethylsilyl]-β-D-ribofuranosyl]-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



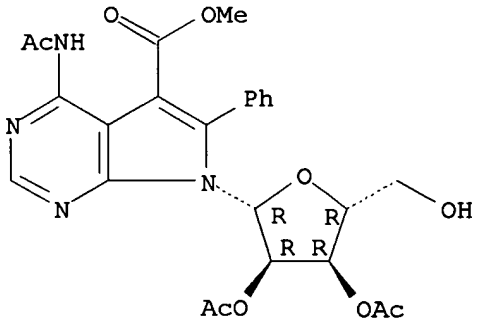
RN 547754-23-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-β-D-ribofuranosyl)-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



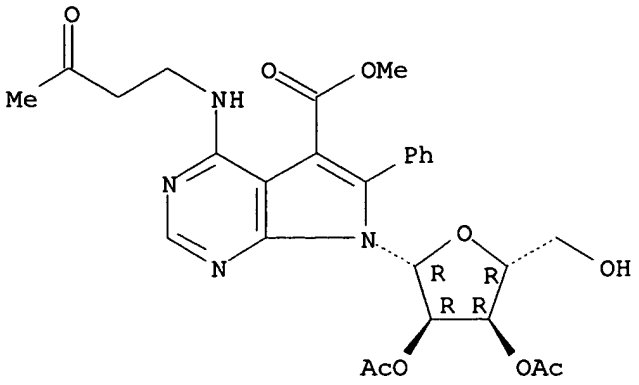
RN 547754-23-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-(acetylamino)-7-(2,3-di-O-acetyl-β-D-ribofuranosyl)-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



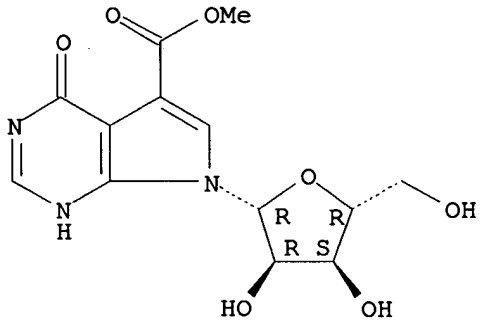
RN 547754-24-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-(2,3-di-O-acetyl-β-D-ribofuranosyl)-4-[(3-oxobutyl)amino]-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



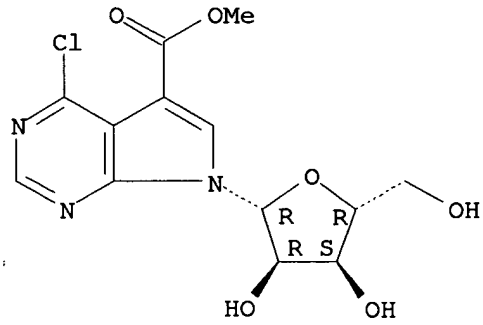
RN 547754-37-0 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



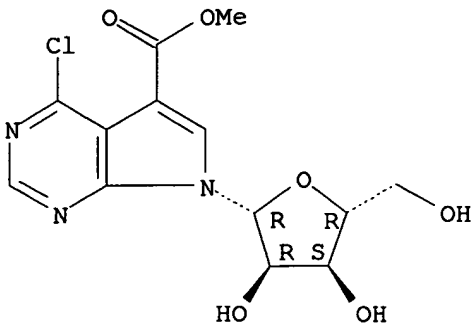
RN 547754-38-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



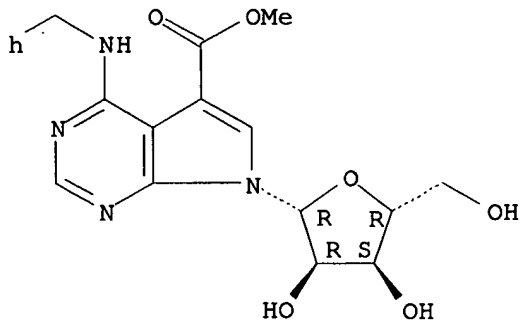
RN 547754-38-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 547754-39-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-[(phenylmethyl)amino]-7-β-D-ribofuranosyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:202427 CAPLUS
DOCUMENT NUMBER: 138:221789
TITLE: Preparation of dioxolane and oxathiolane nucleosides as antivirals and inhibitors of RNA-dependent RNA viral polymerase
INVENTOR(S): Carroll, Steven S.; MacCoss, Malcolm; Kuo, Lawrence C.; Olsen, David B.; Bhat, Balkrishen; Eldrup, Anne Bettina; Prhavc, Marija; Malik, Leila; Bera, Sanjib
PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

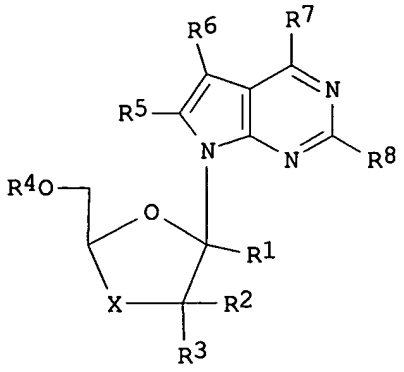
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020222	A2	20030313	WO 2002-US28078	20020829
WO 2003020222	A3	20031127		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-317070P P 20010904

OTHER SOURCE(S): MARPAT 138:221789

GI



I

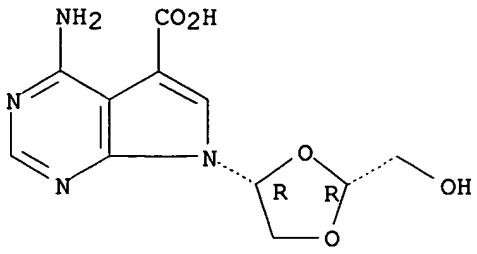
AB The present invention provides 1,3-dioxolane and 1,3-oxathiolane derivs. I, wherein X is O or S(O)n; n is 0-2; R1 is hydrogen, Me, hydroxymethyl, or fluoromethyl; R2 and R3 are each independently hydrogen or alkyl, wherein alkyl is optionally substituted with hydroxy, amino, alkoxy, alkylthio, or one to three halogen atoms; R4 is H, alkylcarbonyl, phosphate; R5 is H, alkyl, alkynyl, halogen, cyano, carboxy, alkyloxycarbonyl, azido, amino, alkylamino, di(alkyl)amino, hydroxy, alkoxy, alkylthio, alkylsulfonyl, aminomethyl; R6 is hydrogen, cyano, nitro, alkyl, NHCONH2, amide, ester, C(=NH)NH2, hydroxy, alkoxy, amino, alkylamino, di(alkyl)amino, halogen, (1,3-oxazol-2-yl), (1,3-thiazol-2-yl), or (imidazol-2-yl); R7 and R8 are each independently hydrogen, hydroxy, halogen, alkoxy, amino, alkylamino, di(alkyl)amino, cycloalkylamino, or di(cycloalkyl)amino; wherein said RNA-dependent RNA viral polymerase is Flaviviridae viral polymerase or Picornaviridae viral polymerase and said RNA-dependent RNA viral replication is Flaviviridae viral replication or Picornaviridae viral replication. These compds. are also inhibitors of RNA-dependent RNA viral replication and are useful in the treatment of RNA-dependent RNA viral infection. The invention also describes pharmaceutical compns. containing such 1,3-dioxolane and 1,3-oxathiolane derivs. alone or in combination with other agents active against RNA-dependent RNA viral infection. Also disclosed are methods of inhibiting RNA-dependent RNA viral polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the compds. of the present invention. Flaviviridae viral polymerase is selected from the group consisting of hepatitis C virus polymerase, yellow fever virus polymerase, dengue virus polymerase, West Nile virus polymerase, Japanese encephalitis virus polymerase, and bovine viral diarrhea virus (BVDV) polymerase. Thus, cis-2-hydroxymethyl-4-(4-amino-5-carboxy-1H-pyrrolo[2,3-d]pyrimidin-7-yl)-1,3-dioxolane was prepared as antiviral agent and inhibitor of RNA-dependent RNA viral polymerase.

IT **501013-62-3P 501013-73-6P 501013-87-2P**
501013-98-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dioxolane and oxathiolane nucleosides as antivirals and inhibitors of RNA-dependent RNA viral polymerase)

RN 501013-62-3 CAPLUS

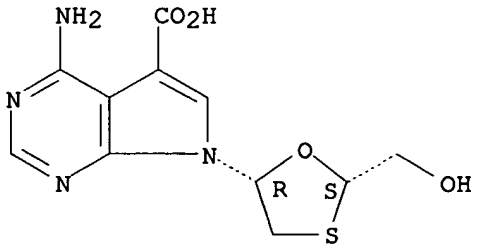
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,4R)-2-(hydroxymethyl)-1,3-dioxolan-4-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



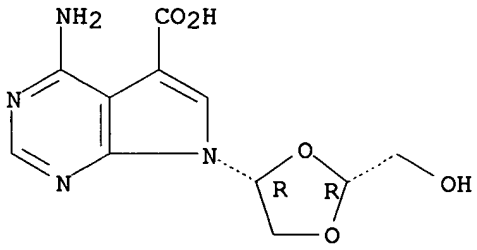
RN 501013-73-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,5S)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



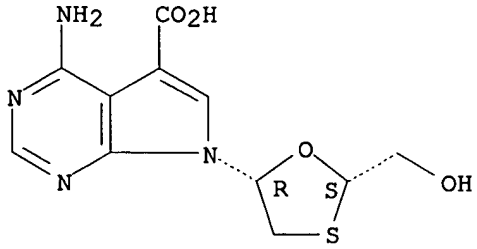
RN 501013-87-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2R,4R)-2-(hydroxymethyl)-1,3-dioxolan-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 501013-98-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[(2S,5R)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 16 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:555629 CAPLUS
DOCUMENT NUMBER: 137:125359
TITLE: Preparation of nucleoside derivatives as inhibitors of

RNA-dependent RNA viral polymerase

INVENTOR(S): Carroll, Steven S.; Lafemina, Robert L.; Hall, Dawn L.; Himmelberger, Amy L.; Kuo, Lawrence C.; Maccoss, Malcolm; Olsen, David B.; Rutkowski, Carrie A.; Tomassini, Joanne E.; An, Haoyun; Bhat, Balkrishen; Bhat, Neelima; Cook, Phillip Dan; Eldrup, Anne B.; Guinosso, Charles J.; Prhavc, Marija; Prakash, Thazha P.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 235 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

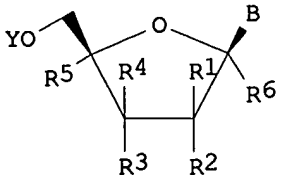
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057425	A2	20020725	WO 2002-US1531	20020118
WO 2002057425	A3	20050421		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2433878	AA	20020725	CA 2002-2433878	20020118
US 2002147160	A1	20021010	US 2002-52318	20020118
US 6777395	B2	20040817		
CN 1498221	A	20040519	CN 2002-806977	20020118
JP 2004532184	T2	20041021	JP 2002-558479	20020118
EP 1539188	A2	20050615	EP 2002-709095	20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004072788	A1	20040415	US 2003-431657	20030507
ZA 2003005078	A	20040521	ZA 2003-5078	20030630
US 2004067901	A1	20040408	US 2003-688691	20031017
US 2004110717	A1	20040610	US 2004-250873	20040116
US 2005272676	A1	20051208	US 2005-200499	20050809

PRIORITY APPLN. INFO.:

US 2001-263313P	P	20010122
US 2001-282069P	P	20010406
US 2001-299320P	P	20010619
US 2001-344528P	P	20011025
US 2002-52318	A3	20020118
WO 2002-US1531	W	20020118
US 2003-431657	B1	20030507

OTHER SOURCE(S): MARPAT 137:125359

GI



I

AB The present invention provides the preparation of nucleoside compds. I, wherein B is nucleobase, Y is H, alkylcarbonyl, phosphate; R1 is H, alkenyl, alkynyl, alkyl; R2 and R3 are independently H, OH, halogen, alkyl, alkoxy, alkenyloxy, alkylthio, alkylcarbonyloxy, aryloxycrbonyl, azido, amino, alkylamino; R1 and R2 together with the carbon atom to which they are attached form a 3- to 6-membered heterocycle; R4 is H, OH, SH, NH2,

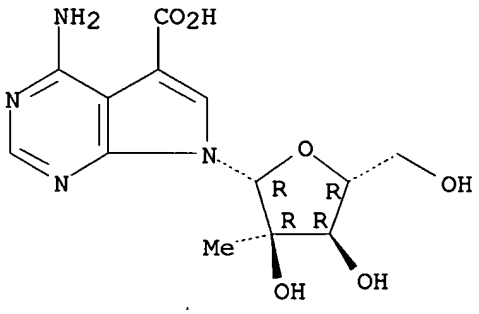
alkylamino, cycloalkylamino, halogen, alkyl, alkoxy, CF3; R5 and R6 are independently H, hydroxymethyl, Me, fluoromethyl; and certain derivs. thereof which are inhibitors of RNA-dependent RNA viral polymerase. These compds. are inhibitors of RNA-dependent RNA viral replication and are useful for the treatment of RNA-dependent RNA viral infection. They are particularly useful as inhibitors of hepatitis C virus (HCV) NS5B polymerase, as inhibitors of HCV replication, and/or for the treatment of hepatitis C infection. The invention also describes pharmaceutical compns. containing such nucleoside compds. alone or in combination with other agents active against RNA-dependent RNA viral infection, in particular HCV infection. Also disclosed are methods of inhibiting RNA-dependent RNA polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the nucleoside compds. of the present invention. Thus, 4-amino-1-(2-C-methyl-β-D-ribofuranosyl)-1H-pyrazolo[3,4-d]pyrimidine was prepared as inhibitors of RNA-dependent RNA viral polymerase. Representative compds. tested in the HCV NS5B polymerase assay exhibited IC's less than 100 μM. The compds. of the present invention were also evaluated for their ability to affect the replication of Hepatitis C Virus RNA in cultured hepatoma (HuH-7) cells containing a sub-genomic HCV Replicon.

IT **443642-56-6P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nucleoside derivs. as inhibitors of RNA-dependent human RNA viral polymerase)

RN 443642-56-6 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 17 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:555511 CAPLUS

DOCUMENT NUMBER: 137:109450

TITLE: Preparation of nucleoside derivatives as inhibitors of RNA-dependent RNA viral polymerase

INVENTOR(S): Carroll, Steven S.; Maccoss, Malcolm; Olsen, David B.; Bhat, Balkrishen; Bhat, Neelima; Cook, Phillip Dan; Eldrup, Anne B.; Prakash, Thazha P.; Prhavc, Marija; Song, Quanlai

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Isis Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057287	A2	20020725	WO 2002-US3086	20020118
WO 2002057287	A3	20021010		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2434386	AA	20020825	CA 2002-2434386		20020118
US 2002147160	A1	20021010	US 2002-52318		20020118
US 6777395	B2	20040817			
EE 200300338	A	20031015	EE 2003-338		20020118
EP 1355916	A2	20031029	EP 2002-709299		20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2002006614	A	20040217	BR 2002-6614		20020118
CN 1498221	A	20040519	CN 2002-806977		20020118
JP 2004520367	T2	20040708	JP 2002-557963		20020118
NZ 526703	A	20041224	NZ 2002-526703		20020118
US 2004072788	A1	20040415	US 2003-431657		20030507
ZA 2003005078	A	20040521	ZA 2003-5078		20030630
BG 108000	A	20040831	BG 2003-108000		20030717
NO 2003003289	A	20030919	NO 2003-3289		20030721
US 2004067901	A1	20040408	US 2003-688691		20031017
US 2005272676	A1	20051208	US 2005-200499		20050809
PRIORITY APPLN. INFO.:			US 2001-263313P	P	20010122
			US 2001-282069P	P	20010406
			US 2001-299320P	P	20010619
			US 2001-344528P	P	20011025
			US 2002-52318	A3	20020118
			WO 2002-US3086	W	20020118
			US 2003-431657	B1	20030507

OTHER SOURCE(S): MARPAT 137:109450

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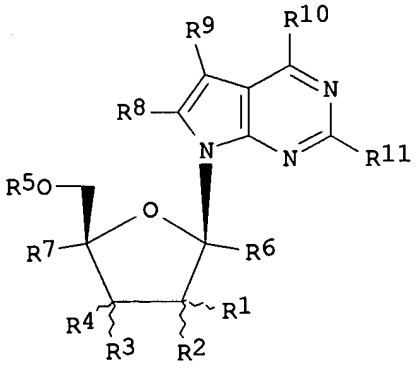


I

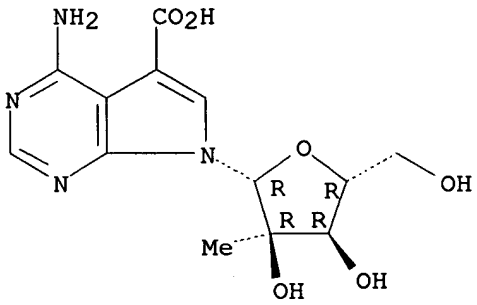
AB The present invention provides nucleoside compds. I, wherein R1 is alkenyl, alkynyl, alkyl, wherein alkyl is unsubstituted or substituted with hydroxy, amino, alkoxy, alkylthio, one to three fluorine atoms; R2 is hydrogen, fluorine, hydroxy, mercapto, alkoxy, alkyl; or R1 and R2 together with the carbon atom to which they are attached form a 3- to 6-membered saturated monocyclic ring system optionally containing a heteroatom selected from O, S, and NC-alkyl; R3 and R4 are each independently hydrogen, cyano, azido, halogen, hydroxy, mercapto, amino, alkoxy, alkenyl, alkynyl, alkyl; R5 is hydrogen, alkylcarbonyl, phosphate; R6 and R7 are each independently hydrogen, Me, hydroxymethyl, or fluoromethyl; R8 is hydrogen, alkyl, alkynyl, halogen, cyano, carboxy, alkyloxycarbonyl, azido, amino, alkylamino, di(alkyl)amino, hydroxy, alkoxy, alkylthio, alkylsulfonyl, alkylaminomethyl, cycloheteroalkyl; R9 is hydrogen, cyano, nitro, alkyl, NHCONH2, amide, thioamide, ester, C(=NH)NH2, hydroxy, alkoxy, amino, alkylamino, di(alkyl)amino, halogen, (1,3-oxazol-2-yl), (1,3-thiazol-2-yl), or (imidazol-2-yl); R10 and R11 are each independently

hydrogen, hydroxy, halogen, alkoxy, amino, alkylamino, di(alkyl)amino, cycloalkylamino, di(cycloalkyl)amino, cycloheteroalkyl, and certain derivs. thereof which are inhibitors of RNA-dependent RNA viral polymerase. These compds. are inhibitors of RNA-dependent RNA viral replication and are useful for the treatment of RNA-dependent RNA viral infection. They are particularly useful as inhibitors of hepatitis C virus (HCV) NS5B polymerase, as inhibitors of HCV replication, and/or for the treatment of hepatitis C infection. The invention also describes pharmaceutical compns. containing such nucleoside compds. alone or in combination with other agents active against RNA-dependent RNA viral infection, in particular HCV infection. Also disclosed are methods of inhibiting RNA-dependent RNA polymerase, inhibiting RNA-dependent RNA viral replication, and/or treating RNA-dependent RNA viral infection with the nucleoside compds. of the present invention. Thus, 4-amino-7-(2-C-methyl-β-D-arabinofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine was prepared as inhibitors of RNA-dependent RNA viral polymerase. Representative compds. tested in the HCV NS5B polymerase assay exhibited IC's less than 100 μM. The nucleoside derivs. were also screened for cytotoxicity against cultured hepatoma (HuH-7) cells containing a sub-genomic HCV Replicon in an MTS cell-based assay.

IT **443642-56-6P 443643-13-8P**
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nucleoside derivs. as inhibitors of RNA-dependent human RNA viral polymerase)

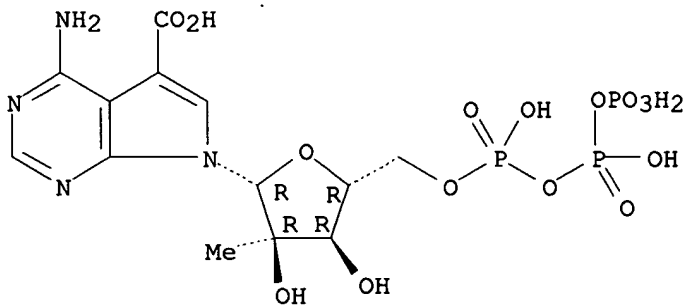
RN 443642-56-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2-C-methyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443643-13-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[5-O-[hydroxy[[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-2-C-methyl-β-D-ribofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



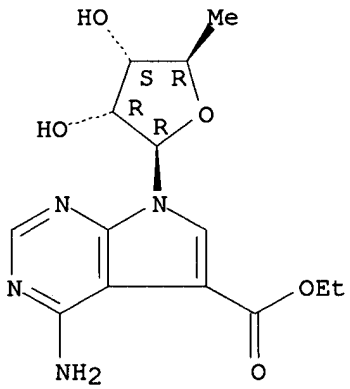
L3 ANSWER 18 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:175767 CAPLUS

DOCUMENT NUMBER: 137:304253
TITLE: QSAR study on adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues using the hansch approach
AUTHOR(S): Srikanth, K.; Debnath, Bikash; Jha, Tarun
CORPORATE SOURCE: Division of Medicinal and Pharmaceutical Chemistry, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, 700032, India
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(6), 899-902
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB QSAR studies on series of pyrrolo[2,3-d]pyrimidine nucleoside analogs were performed for their adenosine kinase (AK) inhibitory activity using the Hansch approach. Significant correlations were obtained with hydrophobic parameter at position 'X'. Electronic and steric parameters on pyrimidine and pyrrole rings found to play an important role in the ligand-receptor interactions with the active sites of the enzyme. Presence of bulkier groups at 'X' and 'Y' positions seems to protect the title compds. from biodegrdn., as is evident from their pos. sterimol steric parameter B1 at these positions.

IT **144928-02-9**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogs using the hansch approach)
RN 144928-02-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:455674 CAPLUS
DOCUMENT NUMBER: 133:222942
TITLE: Adenosine Kinase Inhibitors. 1. Synthesis, Enzyme Inhibition, and Anti-seizure Activity of 5-Iodotubercidin Analogues
AUTHOR(S): Ugarkar, Bheemarao G.; DaRe, Jay M.; Kopcho, Joseph J.; Browne, Clinton E. ,III; Schanzer, Juergen M.; Wiesner, James B.; Erion, Mark D.
CORPORATE SOURCE: Metabasis Therapeutics Inc., San Diego, CA, 92121, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(15), 2883-2893
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:222942

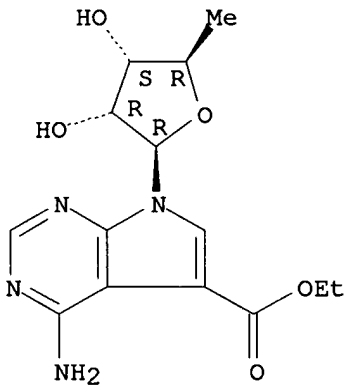
AB Adenosine receptor agonists produce a wide variety of therapeutically useful pharmacologies. However, to date they have failed to undergo successful clin. development due to dose-limiting side effects. Adenosine kinase inhibitors (AKIs) represent an alternative strategy, since AKIs may raise local adenosine levels in a more site- and event-specific manner and thereby elicit the desired pharmacol. with a greater therapeutic window. Starting with 5-iodotubercidin (IC50 = 0.026 μM) and 5'-amino-5'-deoxyadenosine (IC50 = 0.17 μM) as lead inhibitors of the isolated human AK, a variety of pyrrolo[2,3-d]pyrimidine nucleoside analogs were designed and prepared by coupling 5-substituted-4-chloropyrrolo[2,3-d]pyrimidine bases with ribose analogs using the sodium salt-mediated glycosylation procedure. 5'-Amino-5'-deoxy analogs of 5-bromo- and 5-iodotubercidins were found to be the most potent AKIs reported to date (IC50s < 0.001 μM). Several potent AKIs were shown to exhibit anticonvulsant activity in the rat maximal elec. shock (MES) induced seizure assay.

IT **144928-02-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, enzyme inhibition, and anti-seizure activity of iodotubercidin analogs)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

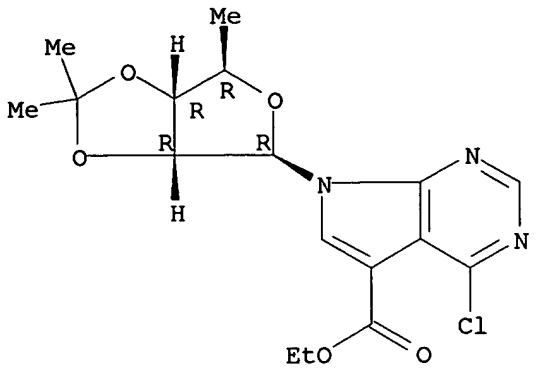


IT **291535-42-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, enzyme inhibition, and anti-seizure activity of iodotubercidin analogs)

RN 291535-42-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-chloro-7-[5-deoxy-2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

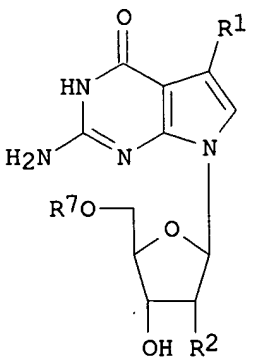


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

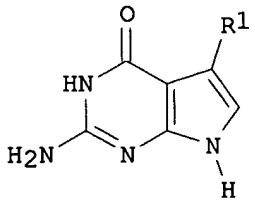
L3 ANSWER 20 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:629981 CAPLUS
DOCUMENT NUMBER: 129:260742
TITLE: Preparation of 7-deaza-2'-deoxyguanosine-5'-triphosphate derivatives and their use in DNA sequencing
INVENTOR(S): Fuller, Carl; McDougall, Mark; Kumar, Shiv
PATENT ASSIGNEE(S): Amersham Pharmacia Biotech Inc, USA
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 866070	A1	19980923	EP 1998-301727	19980309
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
GB 2323357	A1	19980923	GB 1998-5000	19980309
GB 2323357	B2	19990929		
JP 2000119296	A2	20000425	JP 1998-72317	19980320
US 6906185	B1	20050614	US 1998-45732	19980320
PRIORITY APPLN. INFO.:			US 1997-41320P P	19970320

OTHER SOURCE(S): MARPAT 129:260742
GI



I



II

AB The title compds. (I; R1 = C1-10 alkyl optionally substituted with OH, amino, C1-4 alkoxy or halo; R2 = H, OH; R7 = H, mono-, di-, triphosphate

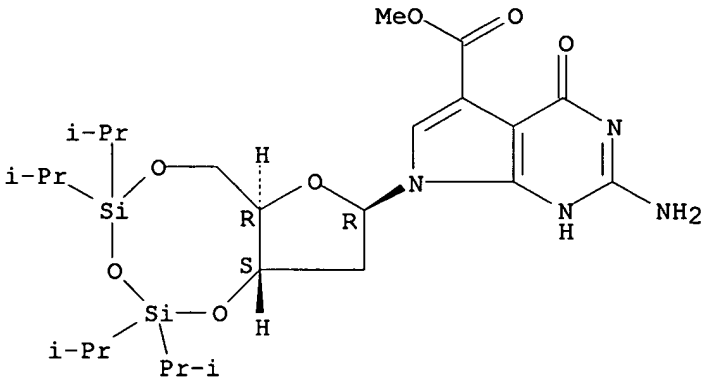
or thiophosphate group; when R1 = Me then R7 ≠ H), useful, e.g., in resolution of compression artifacts in DNA sequencing, were prepared A nucleotide sequence containing I, a DNA acid sequence containing a base II (R1 = C1-10 alkyl, optionally substituted by OH, amino, C1-4 alkoxy or halo), a method for determining the nucleoside base sequence of a DNA mol., a method of elongation of an oligonucleotide sequence, and 7-alkynyl analogs of I are also claimed. For example, esterification of 7-(prop-1-ynyl)-7-deaza-2'-deoxyguanosine and hydrogenation of the resulting 5'-triphosphate ester Et3N-salt with H in the presence of Pd/C gave I (R1 = Pr, R2 = H, R7 = triphosphate group), useful for the title purpose.

IT **213623-53-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 7-deaza-2'-deoxyguanosine-5'-triphosphate derivs. and their use in DNA sequencing)

RN 213623-53-1 CAPLUS

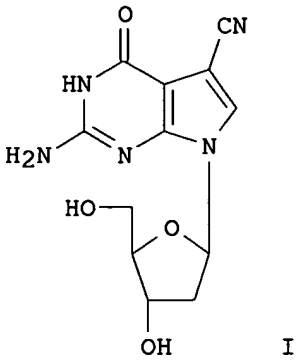
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-[2-deoxy-3,5-O-[1,1,3,3-tetrakis(1-methylethyl)-1,3-disiloxanediyl]-β-D-erythro-pentofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:600335 CAPLUS
DOCUMENT NUMBER: 129:316495
TITLE: Facile synthesis of 2'-deoxynucleoside analogs of preQ
AUTHOR(S): Ramzaeva, Natalya; Becher, Georg; Seela, Frank
CORPORATE SOURCE: Laboratorium Organische Bioorganische Chemie, Institut Chemie, Universitaet Osnabrueck, Osnabrueck, D-49069, Germany
SOURCE: Synthesis (1998), (9), 1327-1330
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

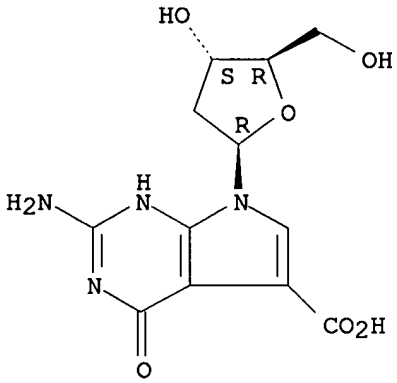
AB The 2'-deoxy derivative of the naturally occurring preQ0 nucleoside I as well as its pyrazolo[3,4-d]pyrimidine analog were synthesized by Cu-mediated cyanation of the corresponding 7-iodo-7-deazaguanine or -8-azaguanine nucleoside. The compds. were converted into the corresponding 7-carboxy 7-carbamoyl derivs.

IT **124738-85-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deoxynucleoside analogs of preQ)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 22 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:102691 CAPLUS

DOCUMENT NUMBER: 124:261553

TITLE: New synthetic routes to 5-substituted pyrrolo(2,3-d)pyrimidines. total synthesis of rigidin and 2'-deoxy-cadeguomycin. synthesis and characterization of novel mesoionic imidazo(1,2-c)pyrimidine-3-ones

AUTHOR(S): Wei, Yuan

CORPORATE SOURCE: Utah State Univ., Logan, UT, USA

SOURCE: (1995) 138 pp. Avail.: Univ. Microfilms Int., Order No. DA9603501
From: Diss. Abstr. Int., B 1995, 56(9), 4894

DOCUMENT TYPE: Dissertation

LANGUAGE: English

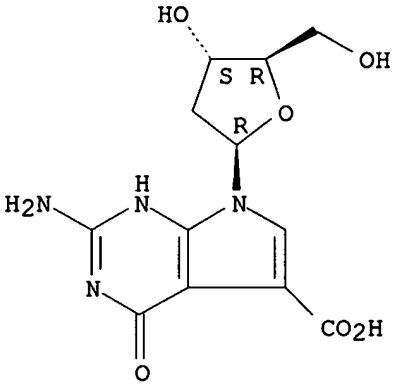
AB Unavailable

IT **124738-85-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of rigidin and deoxycadeguomycin and preparation and characterization of mesoionic imidazopyrimidinones)

RN 124738-85-8 CAPLUS

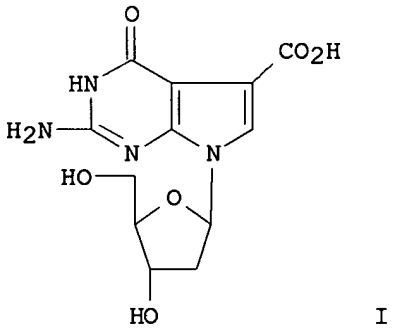
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 23 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:714164 CAPLUS
DOCUMENT NUMBER: 123:83913
TITLE: A New Synthetic Route to β-2'-Deoxyribosyl-5-Substituted Pyrrolo[2,3-d]pyrimidines. Synthesis of 2'-Deoxycadeguomycin
AUTHOR(S): Edstrom, Eric D.; Wei, Yuan
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Utah State University, Logan, UT, 84322-0300, USA
SOURCE: Journal of Organic Chemistry (1995), 60(16), 5069-76
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

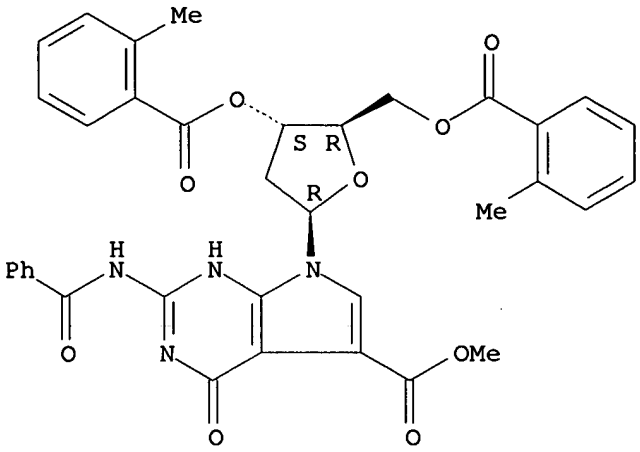


I

AB A new and flexible synthetic route to β-2'-deoxyribosyl-5-substituted pyrrolo[2,3-d]pyrimidines has been developed. Formation of the pyrrole ring is effected by combining sodium N-(4-nitrophenethyl)glycinate with a differently protected 6-chlorouracil derivative generating a substitution adduct. Heating of this material in acetic anhydride affords the 5-(acetyloxy)pyrrolo[2,3-d]pyrimidine 9 in high yield. Base-mediated removal of the pyrrole protecting group gives free pyrrole 10 which is then glycosylated with 1-chloro-2-deoxy-3,5-ditoluoyl-α-D-erythro-pentofuranose using the sodium salt method. The resulting glycosides 15a,b (α:β, 1:4) are readily separated following hydrolysis of the C-5 acetyloxy group. An efficient synthetic route to the pyrrolo[2,3-d]pyrimidine nucleotide analog, deoxycadeguomycin I, is presented. The key transformation involves the conversion of the differentially protected pyrrolo[2,3-d]pyrimidine-2,4-dione base portion into a protected 2-aminopyrrolo[2,3-d]pyrimidin-4-one.

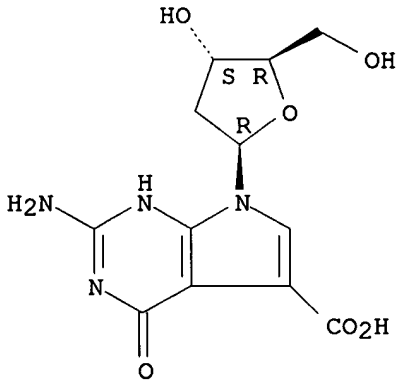
IT **165260-45-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolopyrimidine deoxyribonucleosides and deoxycadeguomycin)
RN 165260-45-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(benzoylamino)-7-[2-deoxy-3,5-bis-O-(2-methylbenzoyl)-β-D-erythro-pentofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



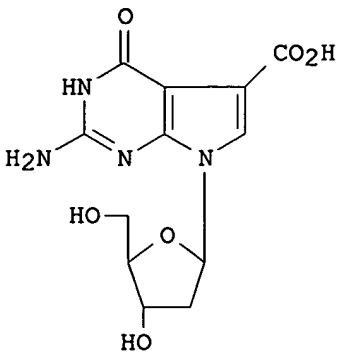
IT **124738-85-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrrolopyrimidine deoxyribonucleosides and deoxycadeguomycin)
RN 124738-85-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 24 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:263070 CAPLUS
DOCUMENT NUMBER: 122:133655
TITLE: Total synthesis of 2'-deoxycadeguomycin, a new pyrrolo[2,3-d]pyrimidine nucleotide analog
AUTHOR(S): Edstrom, Eric D.; Wei, Yuan
CORPORATE SOURCE: Dep. of Chem. and Biochemistry, Utah State Univ., Logan, UT, 84322-0300, USA
SOURCE: Tetrahedron Letters (1994), 35(48), 8989-90
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:133655
GI



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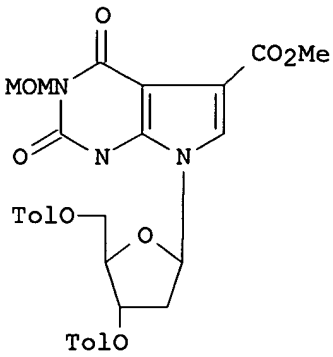


II

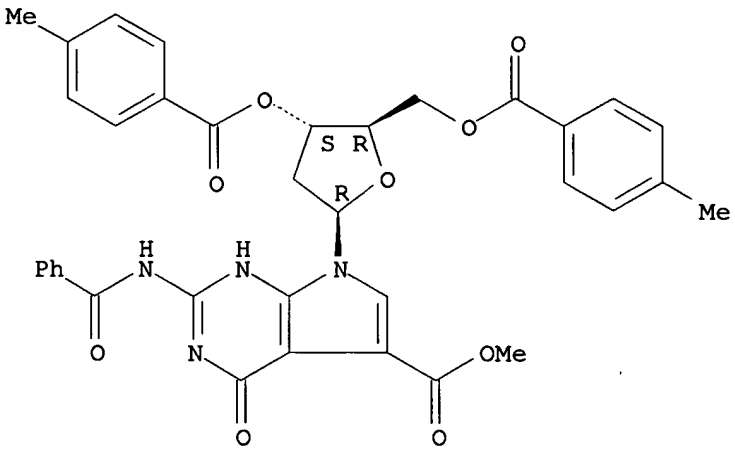
AB This paper describes an efficient synthetic route to a novel pyrrolo[2,3-d]pyrimidine nucleotide analog, 2'-deoxycadeguomycin I. The key transformation involves the conversion of the differentially protected pyrrolo[2,3-d]pyrimidine-2,4-dione base portion in deoxyribonucleoside II into a protected 2-aminopyrrolo[2,3-d]pyrimidin-4-one.

IT **161087-93-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of deoxycadeguomycin from pyrrolopyrimidinedione deoxyribonucleoside via C-2 amination)

RN 161087-93-0 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(benzoylamino)-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

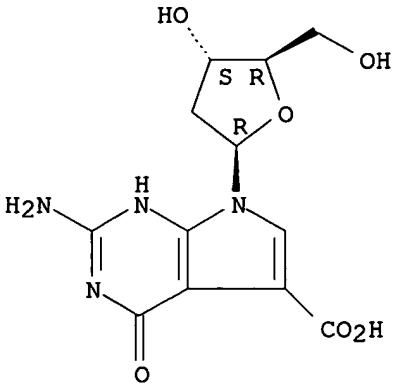


IT **124738-85-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of deoxycadeguomycin from pyrrolopyrimidinedione deoxyribonucleoside via C-2 amination)

RN 124738-85-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

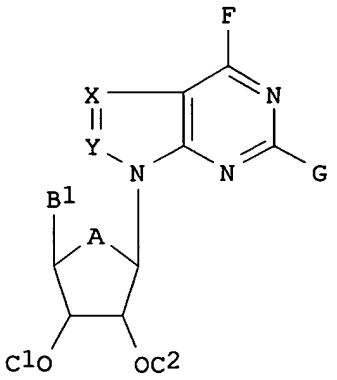
Absolute stereochemistry.



L3 ANSWER 25 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:621999 CAPLUS
DOCUMENT NUMBER: 121:221999
TITLE: Preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents
INVENTOR(S): Firestein, Gary Steven; Ugarkar, Bheemarao Ganapatrao; Miller, Leonard Paul; Gruber, Harry Edward; Bullough, David Andrew; Erion, Mark David; Castellino, Angelo John
PATENT ASSIGNEE(S): Gensia, Inc., USA
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9417803	A1	19940818	WO 1994-US1340		19940203
W: AT, AU, BB, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, UZ					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9462365	A1	19940829	AU 1994-62365		19940203
EP 682519	A1	19951122	EP 1994-909558		19940203
R: CH, DE, FR, GB, IT, LI					
US 5646128	A	19970708	US 1994-349125		19941201
PRIORITY APPLN. INFO.:			US 1993-14190	A	19930203
			US 1989-408707	B2	19890915
			US 1990-466979	B2	19900118
			US 1991-647117	B2	19910123
			US 1991-812916	B2	19911223
			US 1994-192645	B1	19940203
			WO 1994-US1340	W	19940203

OTHER SOURCE(S): MARPAT 121:221999
GI



I

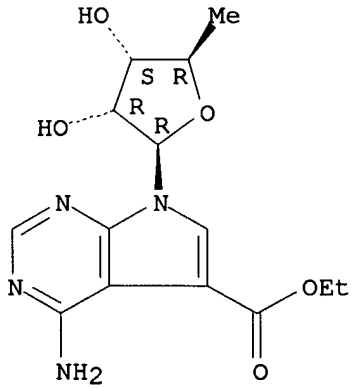
AB Novel nucleosides I [A = O, CH2, S; B' = (CH2)nB, alkenyl, alkynyl; B = H, alkyl, alkoxy, NH2, alkylamino, etc.; C1, C2 = H, acyl, hydrocarbyloxycarbonyl, or C1C2 = C(:O), α-alkoxyalkylidene; X = CD; D = H, halo, alkyl, cyano, CO2H, etc.; Y = N, CE; E = H, halo, alkyl, alkylthio; F = alkyl, aryl, halo, cyano, indolyl, pyrrolidinyl, etc.; G = H, halo, alkyl, alkoxy, alkylamino, alkylthio; n = 1-4], prepared by multistep procedures which are described, selectively inhibit adenosine kinase and are useful in treatment of conditions characterized by an inflammatory response. Such conditions include sepsis, arthritis, autoimmune disease, burns, psoriasis, conjunctivitis, etc. Thus, mice with endotoxemia resulting from injection of Escherichia coli lipopolysaccharide showed a dose-dependent increase in survival in response to i.v. injection of the adenosine kinase inhibitor, 4-amino-1-(5-amino-5-deoxy-1-β-D-ribofuranosyl)-3-bromopyrazolo[3,4-d]pyrimidine-HCl; this effect was antagonized by the adenosine receptor antagonist 8-(p-sulfophenyl)theophylline.

IT **144928-02-9P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of adenosine kinase-inhibiting purine nucleoside analogs as antiinflammatory agents)

RN 144928-02-9 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 26 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:400251 CAPLUS

DOCUMENT NUMBER: 121:251

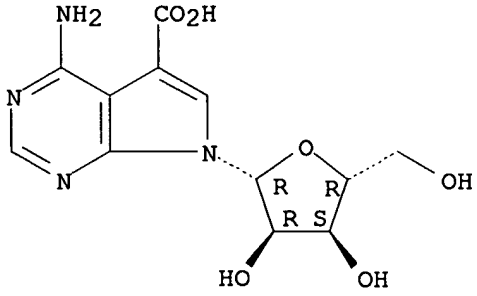
TITLE: Relationship between the structure of sangivamycin-derived nucleosides and their effect on leukemic cell growth and on protein kinase A and C activity

AUTHOR(S): Bobek, Miroslav; Bloch, Alexander
CORPORATE SOURCE: Dep. Exp. Therap., Roswell Park Cancer Inst., Buffalo, NY, 14263, USA
SOURCE: Nucleosides & Nucleotides (1994), 13(1-3), 429-35
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The nucleotide antibiotic sangivamycin (4-amino-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine-5-carboxamide), is an effective inhibitor of protein kinase A (PKA) and protein kinase C (PKC) but, upon its phosphorylation in intact cells, it gains the ability to affect other targets as well. To retain its selectivity for the protein kinases, a series of nonphosphorylatable sangivamycin derivs. was prepared by replacing the 5'-hydroxyl group with other functions including N3, F, SO2NH2, NO2, and NH2,. These derivs. were more potent inhibitors of PKA and PKC than were the phosphorylatable compds., although the latter were more potent inhibitors of leukemic cell growth.

IT **18418-00-3**
RL: BIOL (Biological study)
(antileukemic and protein kinases A and C inhibitory activity of)
RN 18418-00-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

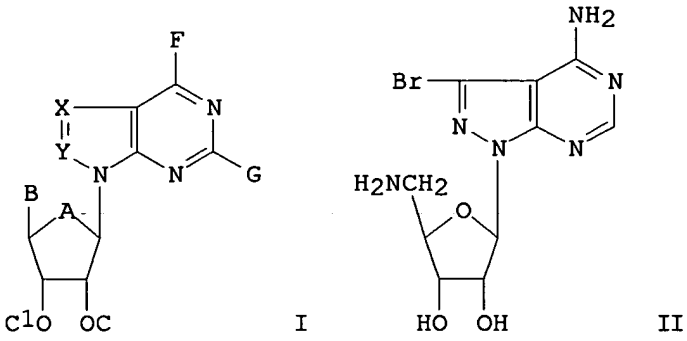


L3 ANSWER 27 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:234420 CAPLUS
DOCUMENT NUMBER: 118:234420
TITLE: Adenosine kinase inhibitors
INVENTOR(S): Browne, Clinton E.; Ugarkar, Bheemarao G.; Mullane, Kevin M.; Gruber, Harry E.; Bullough, David A.; Erion, Mark D.; Castellino, Angelo
PATENT ASSIGNEE(S): Gensia Pharmaceuticals, Inc., USA
SOURCE: Eur. Pat. Appl., 87 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 496617	A1	19920729	EP 1992-300580	19920123
EP 496617	B1	19991201		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE				
CA 2100863	AA	19920724	CA 1992-2100863	19920121
WO 9212718	A1	19920806	WO 1992-US515	19920121
W: AU, CA, FI, NO				
AU 665184	B2	19951221	AU 1992-13599	19920121
AU 9213599	A1	19920827		
JP 05112595	A2	19930507	JP 1992-10094	19920123
IL 100742	A1	19960618	IL 1992-100742	19920123
AT 187175	E	19991215	AT 1992-300580	19920123
NO 9302628	A	19930923	NO 1993-2628	19930721

NO 180418	B	19970106			
NO 180418	C	19970416			
US 5646128	A	19970708	US 1994-349125		19941201
PRIORITY APPLN. INFO.:			US 1991-647117	A	19910123
			US 1991-812916	A	19911223
			US 1989-408707	B2	19890915
			US 1990-466979	B2	19900118
			WO 1992-US515	W	19920121
			US 1993-14190	B2	19930203
			US 1994-192645	B1	19940203

OTHER SOURCE(S): MARPAT 118:234420
GI

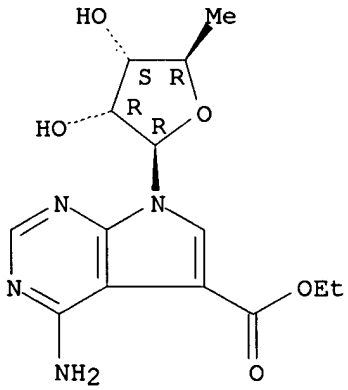


I II

AB Nucleoside analogs I [A = O, CH2, S; B = (un)substituted C1-4 alkyl; C, C1 = H, protective group(s); X = (un)substituted CH; Y = N, (un)substituted CH; F = alkyl, aryl, aralkyl, halogen, (un)substituted NH2, substituted OH or SH, cyano, cyanoalkyl; G = H, halogen, alkyl, alkoxy, alkylamino, alkylthio] were prepared Thus, the analog II was prepared from the pyrimidinone via the azide. II has an adenosine kinase-inhibiting ED50 of <10 nM and was effective in improving post-ischemic functional recovery in isolated guinea pig heart and in preclin. angina models.

IT **144928-02-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 144928-02-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(5-deoxy-β-D-ribofuranosyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 28 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:33911 CAPLUS
DOCUMENT NUMBER: 116:33911

TITLE: Structure-activity relationships for cadeguomycin analogs

AUTHOR(S): Kim, Sun Hee; Okazaki, Kimitake; Okabe, Takayoshi; Nishimura, Toshio; Kondo, Tadao; Tanaka, Nobuo; Suzuki, Hideo

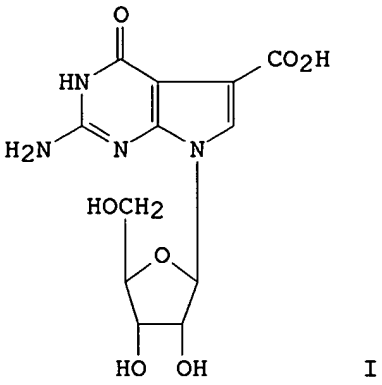
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Antibiotics (1991), 44(6), 659-64
CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

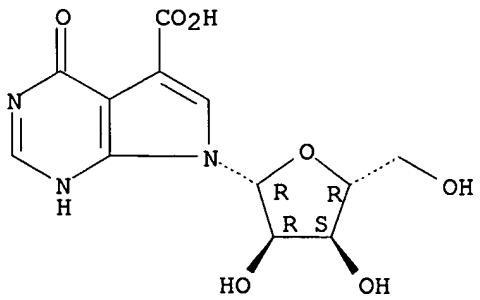
AB The relationship between the antitumor activity and the chemical structure of cadeguomycin (CDM, I) was studied with 6 analogs of CDM. Both activities of CDM, enhancing the incorporation of [3H]thymidine in K562 cells and potentiating the cytotoxicity of cytosine arabinoside for K562 cells, were significantly augmented by the replacement of the 7-carboxyl group with cyano (CDM-CN) or formyl (CDM-CHO), but they were not changed by the replacement with Me. The activities were almost completely diminished by the replacement of ribose with arabinose, but the simultaneous replacement of carboxyl and ribose with formyl and arabinose showed higher activities than those of CDM. The replacement of 7-carboxy-7-deazaguanine with 7-carboxy-7-deazainosine markedly weakened the activity. CDM-CN and CDM-CHO at 0.2 μg/mL significantly potentiated the activity of cytosine arabinoside against MOLT-3 cells but CDM at 1 μg/mL did not. Thus, the ribose and guanine moieties in the CDM mol. are very important for its activity. Also replacing the carboxyl group at the C-7 position with cyano or formyl group is a useful way to strengthen the CDM activity. These compds. would effectively potentiate cytosine arabinoside against various kinds of tumor cells which CDM could not do.

IT **28070-52-2 81645-08-1 81645-08-1D,**
Cadeguomycin, analogs **104846-27-7**
RL: BIOL (Biological study)
(ara-C cytotoxicity potentiation by, structure in relation to)

RN 28070-52-2 CAPLUS

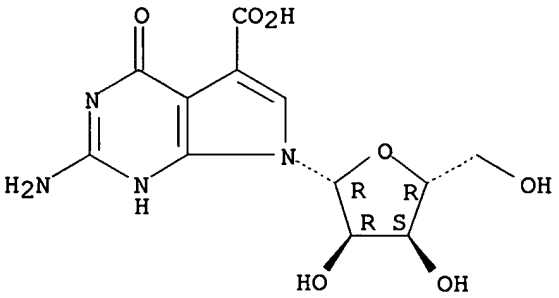
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



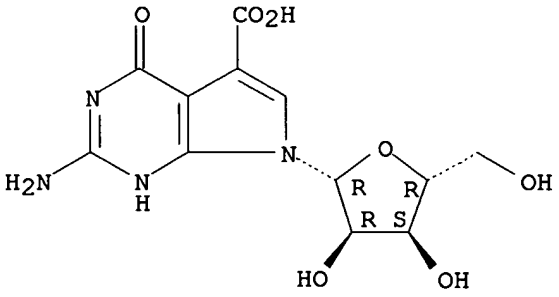
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



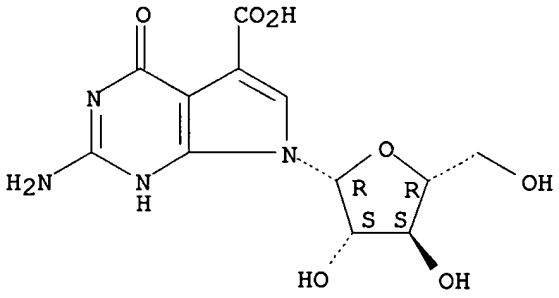
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



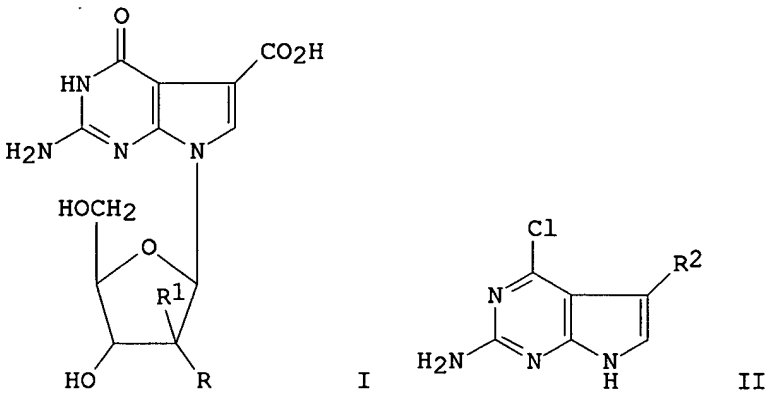
RN 104846-27-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 29 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:217442 CAPLUS
DOCUMENT NUMBER: 112:217442
TITLE: Total and stereospecific synthesis of cadeguomycin, 2'-deoxycadeguomycin, ara-cadeguomycin, and certain related nucleosides
AUTHOR(S): Ramasamy, Kandasamy; Joshi, Ramachandra V.; Robins, Roland K.; Revankar, Ganapathi R.
CORPORATE SOURCE: Dep. Med. Chem., ICN Nucl. Acid Res. Inst., Costa Mesa, CA, 92626, USA
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999)

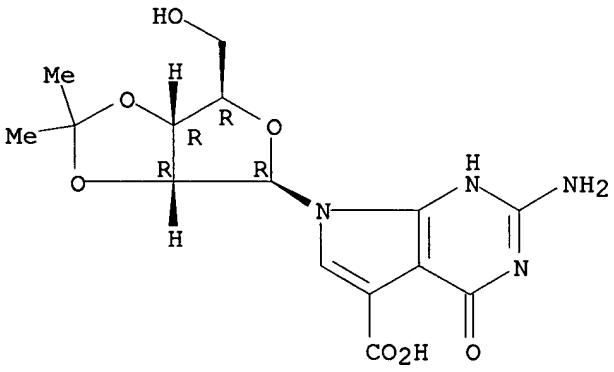
(1989), (12), 2375-84
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:217442
GI



AB A total and stereospecific synthesis of the title cadeguomycins I (R = OH, R1 = H; R = R1 = H; R = H, R1 = OH) was accomplished from the novel aglycons II (R2 = cyano, CO2Me). Ring annulation of 2,6-diaminopyrimidin-4(3H)-one with Me chloro(formyl)acetate in the presence of NaOAc provided a mixture of two products from which the desired Me 2-amino-3,4-dihydro-4-oxo-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylate was separated and converted into II. Several 2-amino-4,5-disubstituted pyrrolo[2,3-d]pyrimidine nucleosides were also prepared

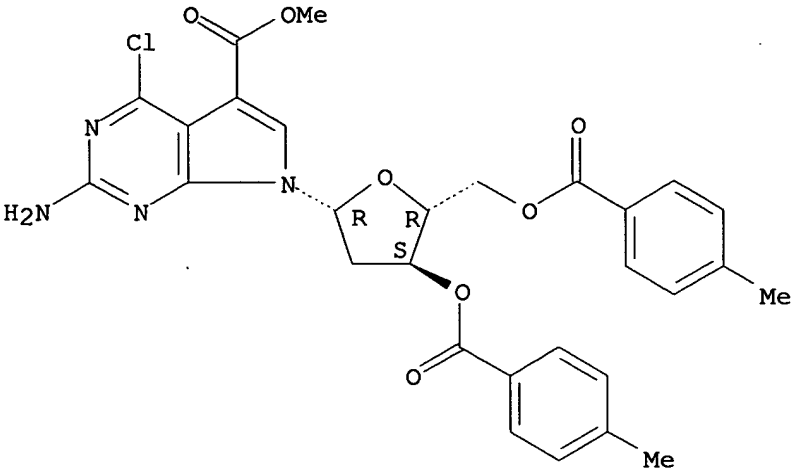
IT **127070-81-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to cadeguomycin)
RN 127070-81-9 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-7-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



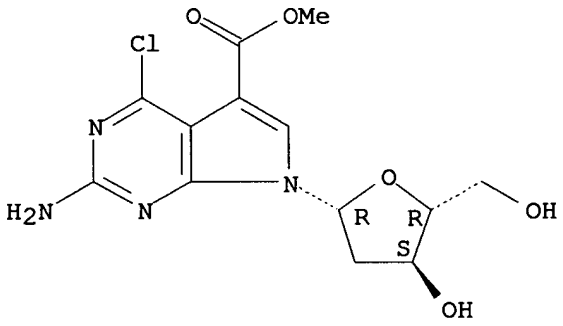
IT **124738-86-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to deoxycadeguomycin)
RN 124738-86-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



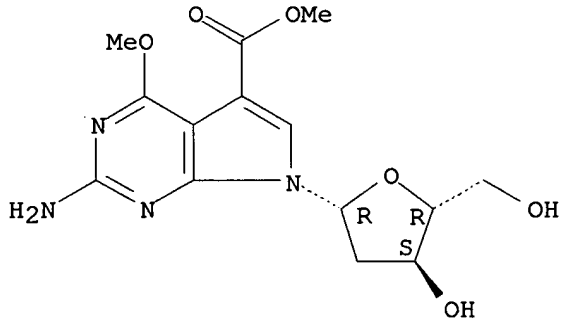
IT **127047-55-6P 127047-56-7P 127047-57-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 127047-55-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-(2-deoxy-β-D-erythro-pentofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



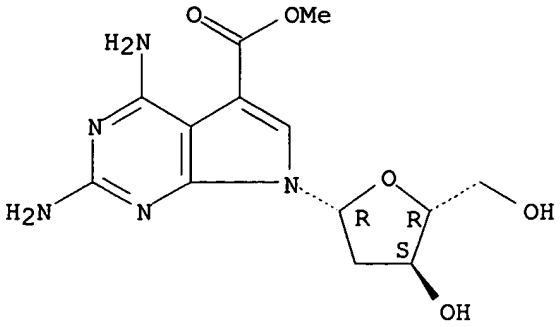
RN 127047-56-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



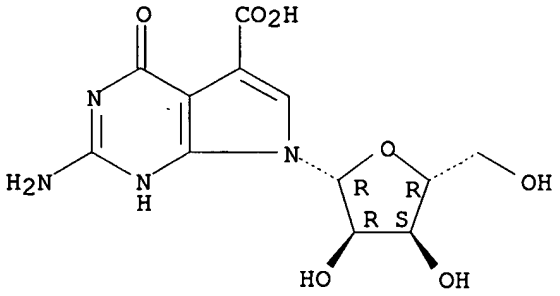
RN 127047-57-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2,4-diamino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



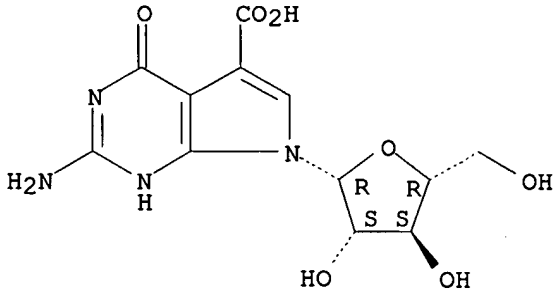
IT **81645-08-1P**, Cadeguomycin **104846-27-7P**, ara-Cadeguomycin
124738-85-8P, 2'-Deoxycadeguomycin
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(total stereospecific synthesis of)
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



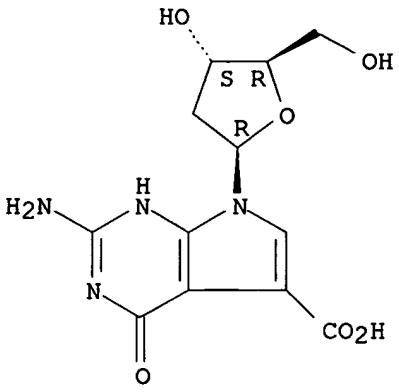
RN 104846-27-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

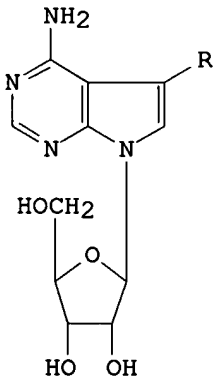


RN 124738-85-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 30 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:155489 CAPLUS
DOCUMENT NUMBER: 112:155489
TITLE: The isolation and structure of modified bioactive nucleosides from Jaspis johnstoni
AUTHOR(S): Zabriskie, T. Mark; Ireland, Chris M.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA
SOURCE: Journal of Natural Products (1989), 52(6), 1353-6
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

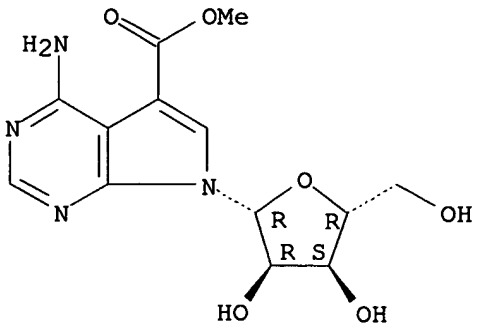


I, R=CN
II, R=CO_2Me

AB Two cytotoxic pyrrolo[2,3-d]pyrimidine nucleosides, toyocamycin (I) and 5-(methoxycarbonyl)tubercidin (II) were isolated from the Fijan sponge J. johnstoni. The structures were solved primarily by 13C-NMR and mass spectral methods and confirmed by comparison to reported values in the literature. Small amts. of the corresponding aglycons were also isolated.

IT **18440-68-1**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge)
RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.

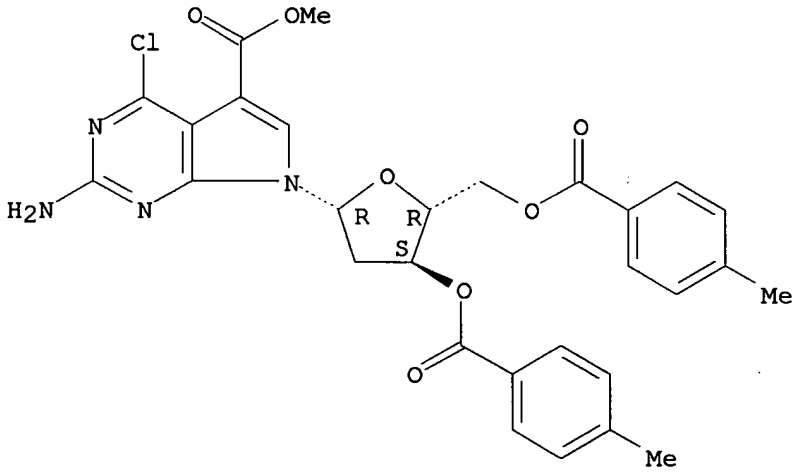


L3 ANSWER 31 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:56513 CAPLUS
DOCUMENT NUMBER: 112:56513
TITLE: Total and stereospecific synthesis of 2'-deoxycadeguomycin
AUTHOR(S): Ramasamy, Kandasamy; Robins, Roland K.; Revankar, Ganapathi R.
CORPORATE SOURCE: Dep. Med. Chem., ICN Nucl. Acid Res. Inst., Costa Mesa, CA, 92626, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1989), (9), 560-2
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:56513

AB An efficient and stereospecific synthesis of 2'-deoxycadeguomycin from both 7-deazapurine derivs. 2-amino-4-chloropyrrolo[2,3-d]pyrimidine-5-carbonitrile and Me 2-amino-4-chloropyrrolo[2,3-d]pyrimidine-5-carboxylate has been accomplished.

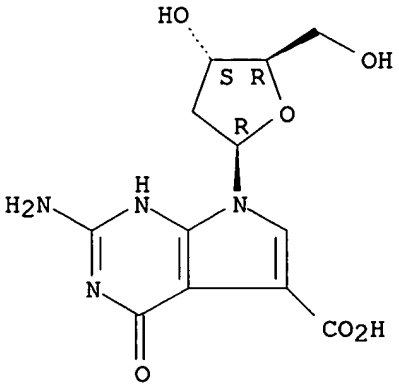
IT **124738-86-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to deoxycadeguomycin)
RN 124738-86-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4-chloro-7-[2-deoxy-3,5-bis-O-(4-methylbenzoyl)-β-D-erythro-pentofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **124738-85-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124738-85-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-deoxy-β-D-erythro-pentofuranosyl)-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

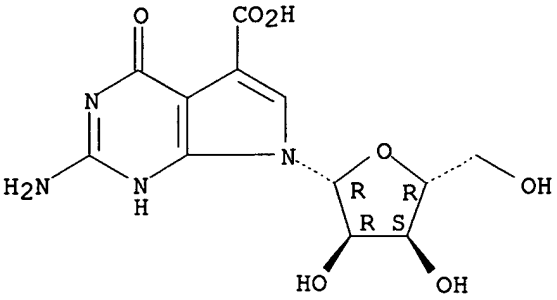


L3 ANSWER 32 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:147191 CAPLUS
DOCUMENT NUMBER: 110:147191
TITLE: Comparative studies of the inhibitory properties of antibiotics on human immunodeficiency virus and avian myeloblastosis virus reverse transcriptases and cellular DNA polymerases
AUTHOR(S): Take, Yukinori; Inouye, Yoshio; Nakamura, Shoshiro; Allaudeen, H. S.; Kubo, Akinori
CORPORATE SOURCE: Sch. Med., Hiroshima Univ., Hiroshima, 734, Japan
SOURCE: Journal of Antibiotics (1989), 42(1), 107-115
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English

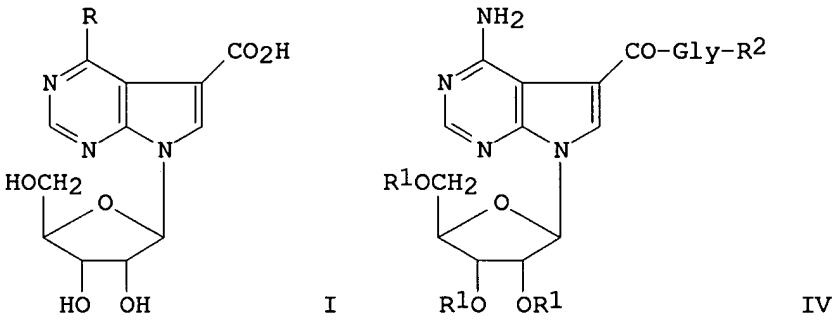
AB The inhibition of human immunodeficiency virus (HIV) reverse transcriptase by certain antibiotics and related compds. was studied in comparison with that of avian myeloblastosis virus (AMV) reverse transcriptase and cellular DNA polymerases α and β. In general, compds. that inhibited HIV reverse transcriptase also inhibited AMV reverse transcriptase. For example, 10 μg/mL of the isoquinoline quinones used in this study inhibited approx. 80% of the activity of reverse transcriptases of HIV and AMV, but did not inhibit the activity of DNA polymerases α and β even at 50 μg/mL. AMV enzyme was more sensitive than HIV enzyme to colistin, enduracidins A and B, janiemycin, glysperin A, and thielavins A and B. The streptonigrin alkyl esters, however, inhibited HIV reverse transcriptase only. Sakyomicin A, luzopeptins, ellagic acid and suramine inhibited the activities of reverse transcriptases and cellular DNA polymerases. Structure-activity relations are discussed.

IT **81645-08-1**, Cadeguomycin
RL: BIOL (Biological study)
(DNA polymerase and human immunodeficiency virus and avian myeloblastosis virus reverse transcriptase inhibition by, structure in relation to)
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 33 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:590805 CAPLUS
DOCUMENT NUMBER: 109:190805
TITLE: Nucleoside peptides. IX. Synthesis of peptide derivatives of sangivamycic acid and deaminosangivamycic acid
AUTHOR(S): Ramasamy, Kandasamy; Robins, Roland K.; Revankar, Ganapathi R.
CORPORATE SOURCE: Dep. Med. Chem., Nucleic Acid Res. Inst., Costa Mesa, CA, 92626, USA
SOURCE: Tetrahedron (1988), 44(4), 1023-34
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:190805
GI

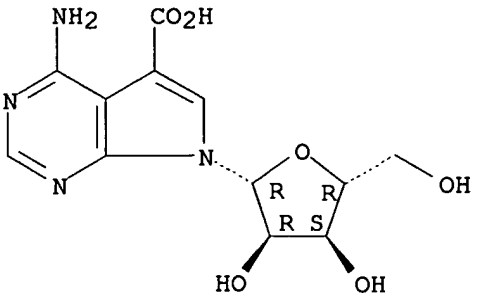


I IV

AB Amino acid and peptide conjugates of sangivamycic acid (I, R = NH2) (II) and deaminosangivamycic acid (I, R = OH) (III) were prepared in which the peptide linkage is on the carboxylic group of the aglycon moiety. The formation of these conjugates was accomplished via coupling of I or II with protected amino acids or peptides mediated by Me2N(CH2)3N:C:NEt.HCl/1-hydroxybenzotriazole. Thus, II was condensed with H-Gly-OEt and then O-acetylated with Ac2O in DMF/pyridine to give nucleoside peptide IV (R1 = Ac, R2 = OEt), which was treated with NH3/MeOH to give IV (R1 = H, R2 = NH2).

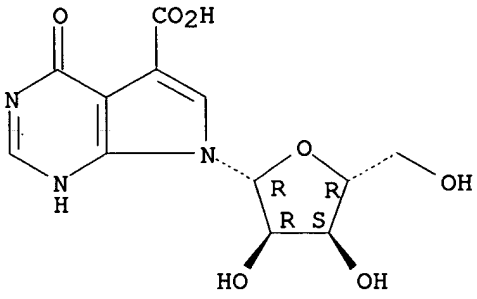
IT **18418-00-3P**, Sangivamycic acid **28070-52-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with amino acids and peptides)
RN 18418-00-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



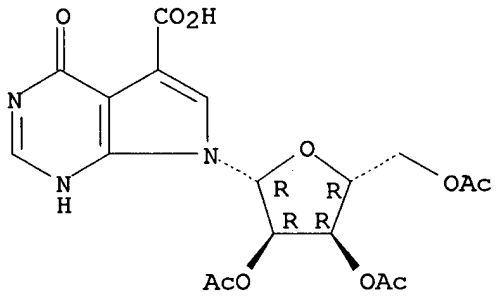
RN 28070-52-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



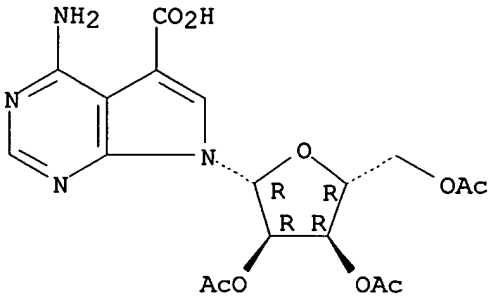
IT **117175-66-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with arginine derivative)
RN 117175-66-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **117175-46-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with glycine Et ester)
RN 117175-46-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

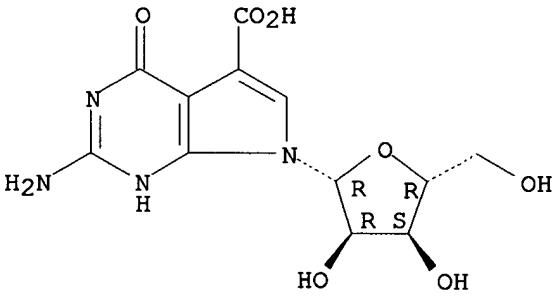


L3 ANSWER 34 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:68455 CAPLUS
DOCUMENT NUMBER: 108:68455
TITLE: Effects of cadeguomycin on cytotoxicity of cytosine arabinoside and other pyrimidine nucleoside analogs; a comparative study
AUTHOR(S): Kim, Sun Hee; Okabe, Takayoshi; Tanaka, Nobuo; Suzuki, Hideo
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Journal of Antibiotics (1987), 40(12), 1776-7
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cadeguomycin at 1 μg/mL did not affect the growth of K562 human myelogenous leukemia cells alone, but it potentiated the cytotoxicity of cytosine arabinoside 56.4-fold and that of 5-fluorodeoxycytidine 10.2-fold. The effects of cadeguomycin on the cytotoxicity of other pyrimidine nucleoside and base analogs were less notable. The decrease of deoxycytidine monophosphate deaminase activity in K562 cells may be related to the neoplasm inhibitor-potentiating effect.

IT **81645-08-1**, Cadeguomycin
RL: BIOL (Biological study)
(neoplasm inhibition by pyrimidine nucleosides increase by, in humans)
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

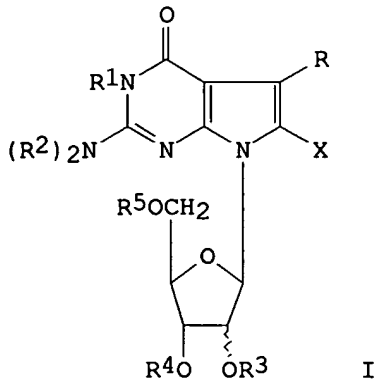
Absolute stereochemistry.



L3 ANSWER 35 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:176807 CAPLUS
DOCUMENT NUMBER: 106:176807
TITLE: 5-Decarboxy-5-formylcadeguomycin analogs
INVENTOR(S): Okamoto, Kaoru; Goto, Toshio; Tanaka, Nobuo
PATENT ASSIGNEE(S): Nippon Zoki Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61229897	A2	19861014	JP 1985-73256	19850405
JP 05060478	B4	19930902		
PRIORITY APPLN. INFO.:			JP 1985-73256	19850405

GI



I

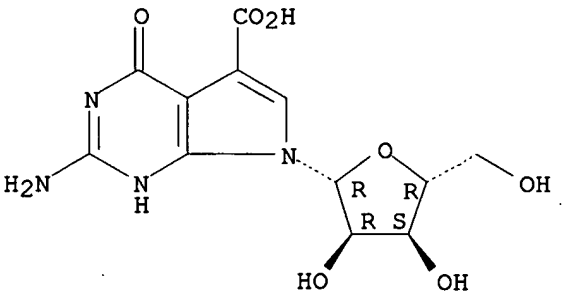
AB The title compound (I; R = CHO; R1-R5 = X = H), useful as an anticancer agent, was prepared Thus, hydrogenolysis of D-ribo-I (R = CH2OH, R1 = CH2OMe, R2 = R5 = Ac, R3R4 = Me2C, X = Br) in aqueous MeOH containing AcOK over Pd/C, oxidation of the resulting D-ribo-I (X = H) in MeCN with MnO2 for 1/2 h followed by ammonolysis and hydrolysis with aqueous CF3CO2H at 70° for 1 h gave D-ribo-I (R = CHO, R1-R5 = X = H). This at 10 μg/mL in vitro inhibited by 50% the growth of mouse lymphatic leukemia L5178Y cells and in vitro enhanced the incorporation of 3H-thymidine into human leukemia K562 cells. Tablets and capsules containing the title compds. were prepared

IT **81645-08-1**, Cadeguomycin
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with methanol)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 36 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1987:131367 CAPLUS
DOCUMENT NUMBER:	106:131367
TITLE:	Potentiation of cytotoxicity of 1-β-D-arabinofuranosylcytosine for K562 Human leukemic cells by cadeguomycin
AUTHOR(S):	Suzuki, Hideo; Kim, Sun Hee; Tahara, Makoto; Okazaki, Kimitake; Okabe, Takayoshi; Wu, Rong Tsun; Tanaka, Nobuo
CORPORATE SOURCE:	Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan
SOURCE:	Cancer Research (1987), 47(3), 713-17 CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal
LANGUAGE: English

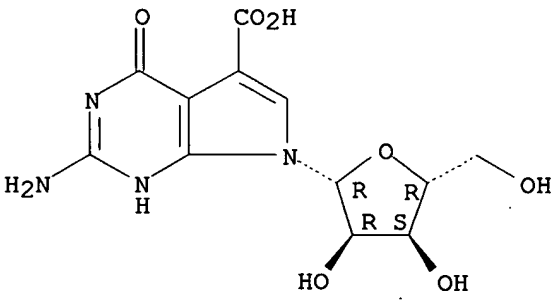
AB The treatment of K562 human myeloblastic leukemia cells and YAC-1 murine lymphoma cells with cadeguomycin [**81645-08-1**] at concns. >0.6 μM significantly enhanced the cytotoxicity of 1-β-D-arabinofuranosylcytosine (ara-C) [147-94-4]. The degree of potentiation depended upon the antibiotic concentration The treatment with 75 μM cadeguomycin for 18 h increased cellular uptake of [3H]ara-C into K562 cells and formation of ara-C nucleotides, as well as incorporation into nucleic acids. The level of the ara-C diphosphate plus the ara-C triphosphate was approx. 10 times higher in the cadeguomycin-treated cells than in the untreated cells by 30 min of incubation with [3H]ara-C. The exts. of 15 μM cadeguomycin-treated K562 cells showed increased activity of formation of ara-C nucleotides, resulting in 4- to 5-fold higher formation of the di- and triphosphates of ara-C than the control cell exts. Cadeguomycin did not significantly change the level of ribonucleotide and deoxyribonucleotide pool in K562 cells. The mechanism of potentiation of ara-C by cadeguomycin is discussed.

IT **81645-08-1**, Cadeguomycin
RL: BIOL (Biological study)
(cytotoxicity of arabinofuranosylcytosine potentiation by)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 37 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:43284 CAPLUS
DOCUMENT NUMBER: 106:43284
TITLE: Studies on substances effective against antitumor drug-resistant tumor cells
AUTHOR(S): Suzuki, Hideo
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan
SOURCE: Medicina Philosophica (1986), 5(8), 646-8
CODEN: MDPHDG; ISSN: 0286-2190
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

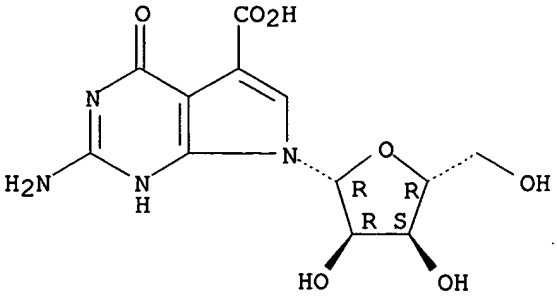
AB A review, with 6 refs., on the mechanism of acquired tolerance of tumor cells to chemotherapeutic agents and the effectiveness of cadeguomycin [**81645-08-1**] and lactoquinomycin A [100100-36-5] against the tolerance when they were obtained with other neoplasm inhibitors.

IT **81645-08-1**
RL: BIOL (Biological study)
(drug resistance to neoplasm inhibitors response to)

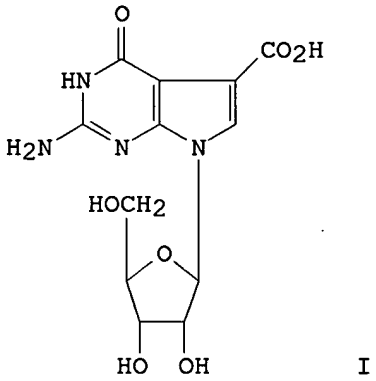
RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 38 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:618445 CAPLUS
DOCUMENT NUMBER: 105:218445
TITLE: Potentiation of arabinosylcytosine-induced erythroid differentiation of human leukemia K562 cells by cadeguomycin
AUTHOR(S): Wu, R. T.; Chen, S. C.; Tien, W. C.; Tanaka, N.
CORPORATE SOURCE: Grad. Program Microbiol. Immunol., Natl. Yang-Ming Med. Coll., Taipei, Taiwan
SOURCE: Recent Adv. Chemother., Proc. Int. Congr. Chemother., 14th (1985), Volume Anticancer Sect. 1, 201-2. Editor(s): Ishigami, Joji. Univ. Tokyo Press: Tokyo, Japan.
CODEN: 55GNAX
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



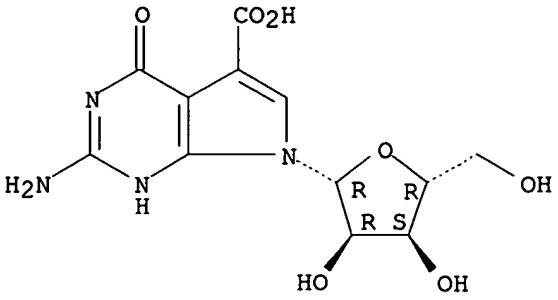
I

AB Cadeguomycin (I) [**81645-08-1**] enhanced the induction of erythroid differentiation in human myelogenous leukemic cells K562 treated with low concns. of ara-C [147-94-4]. In the presence of a low concentration (0.1 μg/mL) of ara-C, I markedly increased the amount of Hb synthesized, up to 20-fold even at a concentration of 1 μg I/mL. The 2 main forms of Hb synthesized by K562 cells in the presence of I and ara-C were Hb Gower-1 [56592-05-3] and Hb Portland [54846-99-0]. After induction of erythroid differentiation by cadeguomycin and ara C, K562 cells lost their clonogenic properties in soft agar medium and tumorigenicity in nude mice.

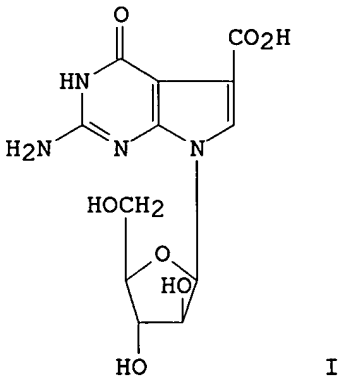
IT **81645-08-1**
RL: BIOL (Biological study)
(arabinosylcytosine-induced erythroid differentiation of human leukemia cell potentiation by)

RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



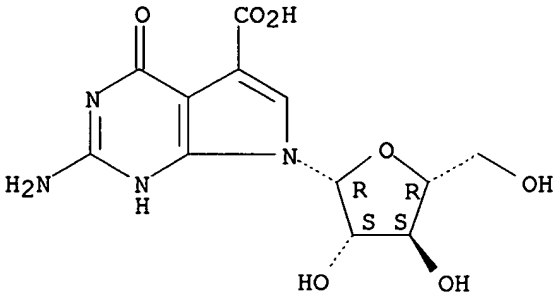
L3 ANSWER 39 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:572961 CAPLUS
DOCUMENT NUMBER: 105:172961
TITLE: Synthesis of ara-cadeguomycin. 2-Amino-3,4-dihydro-4-oxo-7-(β-D-arabinofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid
AUTHOR(S): Okamoto, Kaoru; Kondo, Tadao; Goto, Toshio
CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1986), 59(6), 1915-19
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:172961
GI



I

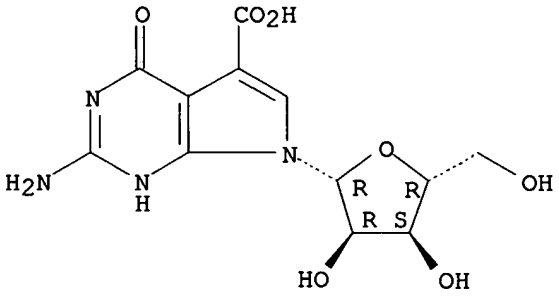
AB The title nucleoside (I), an analog of cadeguomycin, was prepared via glycosylation of 3-methoxymethyl-5-methyl-2-methylthio-7H-pyrrolo[2,3-d]pyrimidin-4(3H)-one with 2,3,5-tri-O-benzyl-D-arabinofuranosyl chloride.
IT **104846-27-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104846-27-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-β-D-arabinofuranosyl-4,7-dihydro-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

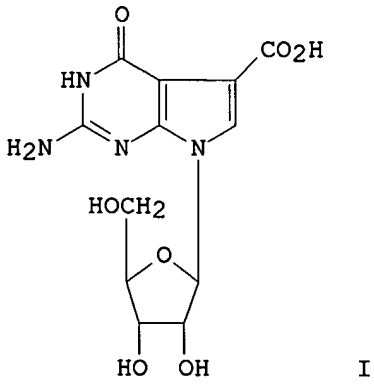


IT **81645-08-1DP**, analog
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of)
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 40 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:497859 CAPLUS
DOCUMENT NUMBER: 105:97859
TITLE: A total synthesis of cadeguomycin, a nucleoside antibiotic produced by Streptomyces hygroscopicus
AUTHOR(S): Kondo, Tadao; Okamoto, Kaoru; Yamamoto, Manabu; Goto, Toshio; Tanaka, Nobuo
CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Tetrahedron (1986), 42(1), 199-205
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:97859
GI



I

AB The nucleoside antibiotic cadeguomycin (I) was prepared from

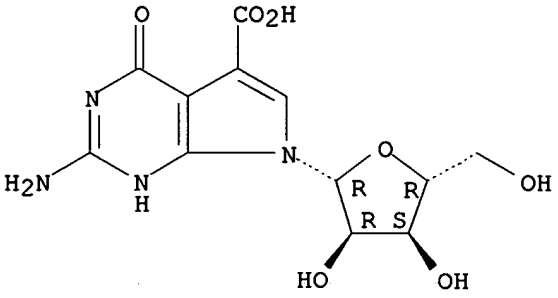
3,4-3-methoxymethyl-5-methyl-2-methylthio-7-(2,3-O-isopropylidene-5-O-triphenylmethyl-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidin-4-one, which was effectively prepared by glycosylation of 3,4-dihydro-3-methoxymethyl-5-methyl-2-methylthio-7H-pyrrolo-[2,3-d]pyrimidin-4-one with 2,3-O-isopropylidene-5-O-triphenylmethyl-β-D-ribofuranosyl chloride.

IT **81645-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 41 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:28534 CAPLUS

DOCUMENT NUMBER: 104:28534

TITLE: Enhancement of pyrimidine nucleoside uptake into K562 and YAC-1 cells by cadeguomycin

AUTHOR(S): Wu, Rong Tsun; Okabe, Takayoshi; Kim, Sun Hee; Suzuki, Hideo; Tanaka, Nobuo

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Journal of Antibiotics (1985), 38(11), 1588-95
CODEN: JANTAJ; ISSN: 0021-8820

DOCUMENT TYPE: Journal

LANGUAGE: English

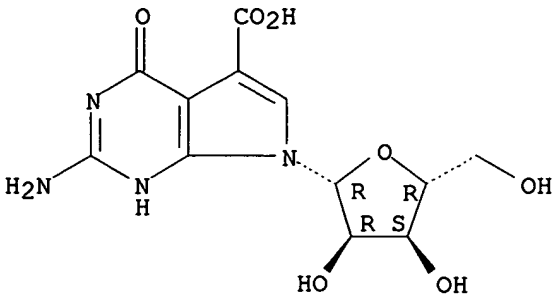
AB Cadeguomycin [**81645-08-1**] markedly stimulated the uptake of thymidine [50-89-5], deoxycytidine [951-77-9], and uridine [58-96-8] into the acid-insol. fraction of K562 human leukemic cells, but did not affect adenosine [58-61-7] incorporation. The enhancement of pyrimidine nucleoside uptake was 6-17-fold over the control. Aspartate incorporation into nucleic acid was not significantly blocked by the antibiotic, suggesting that the stimulation of pyrimidine nucleoside incorporation is not due to the inhibition of de novo pyrimidine nucleotide synthesis. Net DNA and RNA syntheses, observed by [32P]phosphate uptake were not affected by cadeguomycin. The enzymic activity of thymidine kinase [9002-06-6], deoxycytidine kinase [9039-45-6], and uridine kinase [9026-39-5] was higher in cadeguomycin-treated cells than in untreated cells, suggesting that the enhancement of pyrimidine nucleoside uptake occurs in the phosphorylation process. The stimulatory activity of cadeguomycin of thymidine uptake was reversed by guanosine [118-00-3] and deoxyguanosine [961-07-9], but not by adenosine and deoxyadenosine, suggesting that intracellular metabolism and/or action of cadeguomycin is related to that of guanosine and deoxyguanosine. The stimulation of pyrimidine nucleoside incorporation by cadeguomycin was also found with YAC-1 cells, but not with the other cell lines. The enhancement effect of the antibiotic seems to be not directly related to its cytotoxicity.

IT **81645-08-1**
RL: BIOL (Biological study)
(pyrimidine nucleoside uptake by leukemia cells of human enhancement by, kinase activity in relation to)

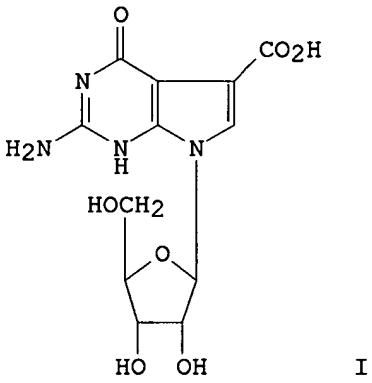
RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 42 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:416522 CAPLUS
DOCUMENT NUMBER: 103:16522
TITLE: Biological activity of cadeguomycin. Inhibition of tumor growth and metastasis, immunostimulation, and potentiation of 1-β-D-arabinofuranosylcytosine
AUTHOR(S): Yuan, Bao Ding; Wu, Rong Tsun; Sato, Isao; Okabe, Takayoshi; Suzuki, Hideo; Nishimura, Toshio; Tanaka, Nobuo
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan
SOURCE: Journal of Antibiotics (1985), 38(5), 642-8
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

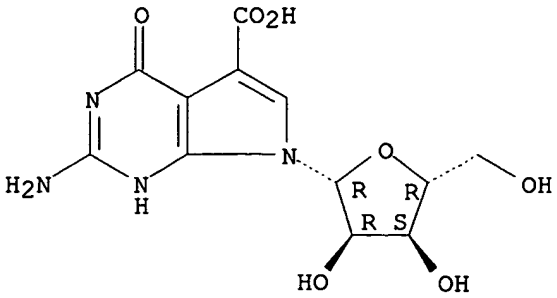
AB Cadeguomycin (I) [**81645-08-1**] retarded the growth of s.c. solid IMC carcinoma and the pulmonary metastasis of Lewis lung carcinoma in mice. The antibiotic enhanced phagocytic activity of murine peritoneal macrophages and interleukin-1 production by P388D1 cells. Delayed-type hypersensitivity was stimulated and interferon was induced by the drug. The results suggest that I inhibits tumor growth and metastasis in association with modification of the immune system. The cytotoxicity of 1-β-D-arabinosylcytosine [147-94-4] to K562 and YAC-1 cells was markedly enhanced by I in culture. The combined administration of arabinosylcytosine and I displayed potentiation of the inhibition of growth of i.p. implanted P388 leukemia and metastasis of s.c. implanted P388 leukemia to the regional lymph nodes. I showed low toxicity in mice.

IT **81645-08-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antineoplastic activity of, metastasis inhibition and immunostimulation and arabinofuranosylcytosine cytotoxicity potentiation in relation to)

RN 81645-08-1 CAPLUS

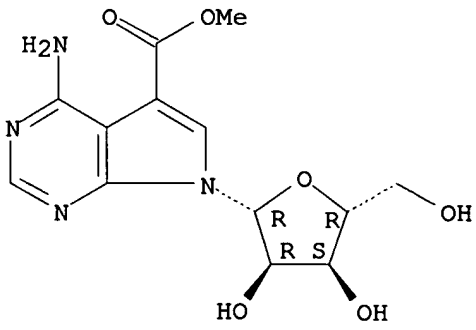
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 43 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:531021 CAPLUS
DOCUMENT NUMBER: 101:131021
TITLE: Fast atom bombardment combined with tandem mass spectrometry for the determination of nucleosides
AUTHOR(S): Crow, Frank W.; Tomer, Kenneth B.; Gross, Michael L.; McCloskey, James A.; Bergstrom, Donald E.
CORPORATE SOURCE: Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588, USA
SOURCE: Analytical Biochemistry (1984), 139(1), 243-62
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The pos. and neg. ion fast atom bombardment (FAB) mass spectra and fast atom bombardment collisionally activated decomposition (CAD) spectra of a series of nucleosides and 2 dinucleotides are reported. The nucleosides studied are substituted forms of guanosine, adenosine, nebularine, tubercidin, uridine, and related pyrimidines. The FAB and CAD data both contain similar information. The CAD spectra provide some structural information not found in the FAB mass spectra. Tandem mass spectrometry also allows emphasis to be put on weak fragments which are either not observed in the FAB mass spectrum or are lost in the matrix ion signals.
IT **18440-68-1**
RL: PRP (Properties)
(fast-atom-bombardment mass spectra and pos.-atom-bombardment tandem mass spectra of)
RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 44 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:103800 CAPLUS
DOCUMENT NUMBER: 100:103800
TITLE: Pyrrolopyrimidine nucleosides. 19. A total synthesis of the nucleoside antibiotic cadeguomycin

[2-amino-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidin-4-one-5-carboxylic acid]

AUTHOR(S): Beylin, Vladimir G.; Kawasaki, Andrew M.; Cheng, Chin Shu; Townsend, Leroy B.

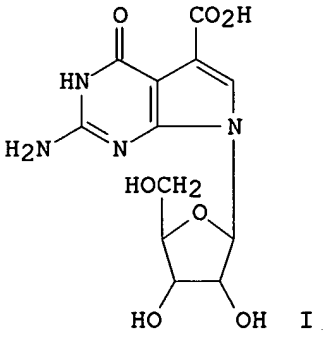
CORPORATE SOURCE: Dep. Med. Chem., Coll. Pharm., Ann Arbor, MI, 48109, USA

SOURCE: Tetrahedron Letters (1983), 24(44), 4793-6
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

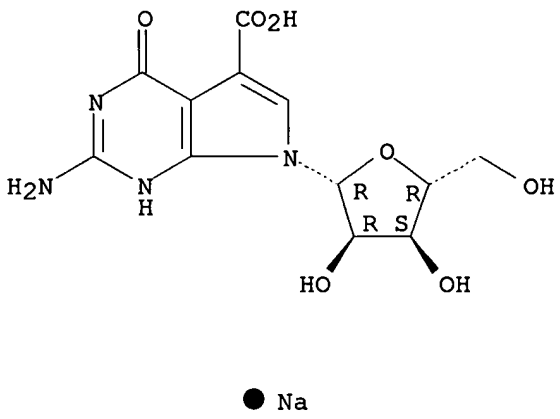
AB A total synthesis of the title nucleoside I was accomplished and confirmed the previous structural assignment for the antibiotic cadeguomycin.

IT **88970-16-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 88970-16-5 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



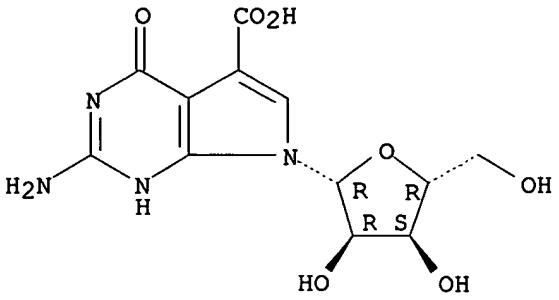
● Na

IT **81645-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

RN 81645-08-1 CAPLUS

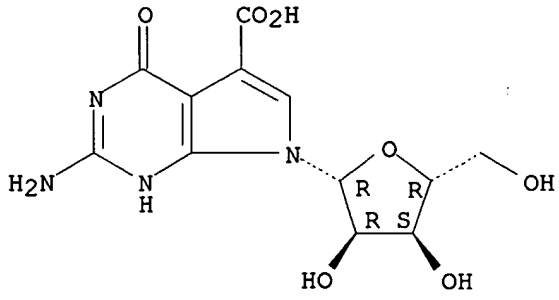
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



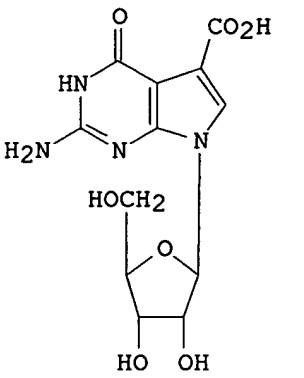
L3 ANSWER 45 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:61483 CAPLUS
DOCUMENT NUMBER: 100:61483
TITLE: Recent studies on mechanism of action of three antitumor antibiotics
AUTHOR(S): Tanaka, Nobuo
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan
SOURCE: Trends Antibiot. Res.: Genet., Biosynth., Actions New Subst., Proc. Int. Conf. (1982), 79-88. Editor(s): Umezawa, Hamao; Demain, Arnold L.; Hata, Toju. Jpn. Antibiot. Res. Assoc.: Tokyo, Japan.
CODEN: 50VJAT
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The mechanism of action of 3 antitumor antibiotics (neothramycin [67298-49-1], 2-crotonyloxymethyl-4,5,6-trihydroxycyclohex-2-enone (COTC) [62532-49-4], and cadeguomycin [**81645-08-1**]) is discussed. Neothramycin binds to the 2-amino group of a guanine base of DNA. COTC is a multifunctional agent affecting many SH-containing substances, DNA polymerase α, and mitotic processes. The mechanism of action of cadeguomycin remains to be clarified, although it seems to involve pyrimidine metabolism
IT **81645-08-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neoplasm-inhibiting activity of, mechanism of)
RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

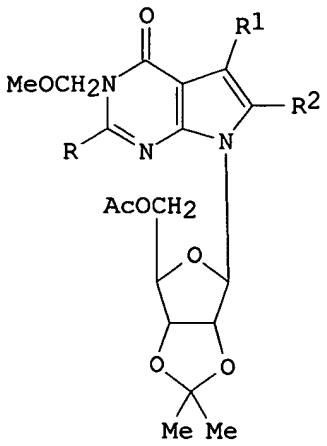


L3 ANSWER 46 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:7038 CAPLUS
DOCUMENT NUMBER: 100:7038
TITLE: Synthesis of cadeguomycin (7-deazaguanosine-7-carboxylic acid)
AUTHOR(S): Kondo, Tadao; Goto, Toshio
CORPORATE SOURCE: Fac. Agric., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Tetrahedron Letters (1983), 24(34), 3647-50

CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

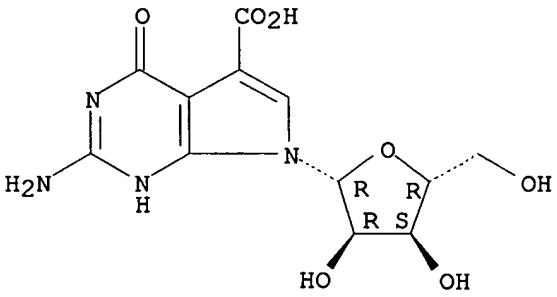
AB Cadeguomycin (I) was prepared from deazaguanosine II (R = Ac2N, R1 = Me, R2 = Br) in 5 steps via α-hydroxylation, oxidation and debromination.

IT **81645-08-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

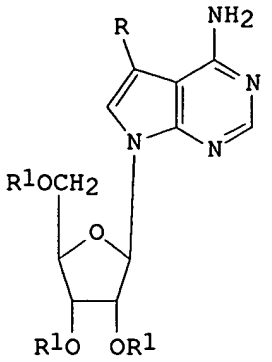
RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 47 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:612871 CAPLUS
DOCUMENT NUMBER: 99:212871
TITLE: Nucleosides and nucleotides. 47. Conversion of tubercidin to toyocamycin: some properties of tubercidin derivatives
AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Nucleosides & Nucleotides (1983), 2(2), 113-25
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

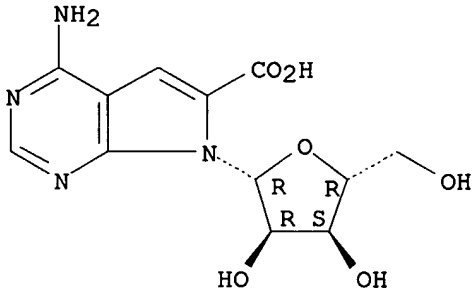
AB Tubercidin (I; R = R1 = H) was converted into toyocamycin (I; R = cyano, R1 = H) in 6 steps via the following sequence of intermediates: I [R, R1 given; (morpholinomethyl), H; (morpholinomethyl), Ac; (1-oxidomorpholinomethyl), Ac; CHO, Ac; and CH:NOH, H]. The NMR and CD spectra of 5- and 6-substituted tubercidins show that 6-substituted tubercidins have the syn-conformation in solution

IT **77049-87-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR and CD of)

RN 77049-87-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 48 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:538171 CAPLUS

DOCUMENT NUMBER: 99:138171

TITLE: Cadeguomycin

PATENT ASSIGNEE(S): Microbiochemical Research Foundation, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

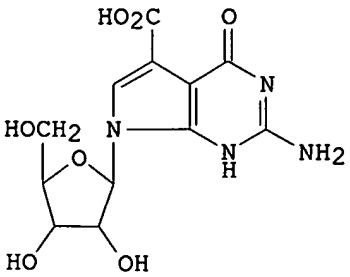
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58092693	A2	19830602	JP 1981-189158	19811127
JP 01039437	B4	19890821		

PRIORITY APPLN. INFO.: JP 1981-189158 19811127

GI



I

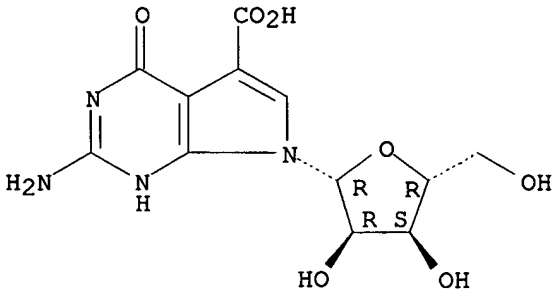
AB Cadeguomycin (I) [**81645-08-1**] was produced by Streptomyces IM791T, freshly isolated from soil and related to S. hygroscopicus ISP5578. Thus, the strain was cultuerd in a medium containing 2% oatmeal and 0.1% yeast extract at 27° for 114 h. The filtrate (90 L) was treated with Amberlite XAD-8 and the eluate fractionated to give 20.8 mg I. I had no antibacterial activity at 100 μg/mL, but enhanced the activity of ara-C [147-94-4] against human leukemia K562 cells.

IT **81645-08-1**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(from Streptomyces)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 49 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:437106 CAPLUS

DOCUMENT NUMBER: 99:37106

TITLE: Antibiotic AB-116

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

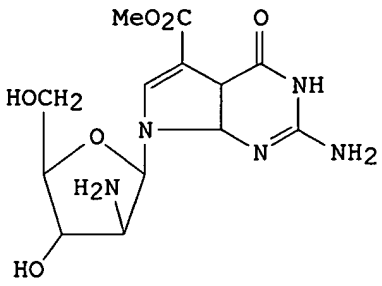
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58032893	A2	19830225	JP 1981-129121	19810817
JP 01053677	B4	19891115		

PRIORITY APPLN. INFO.: JP 1981-129121 19810817

GI



I

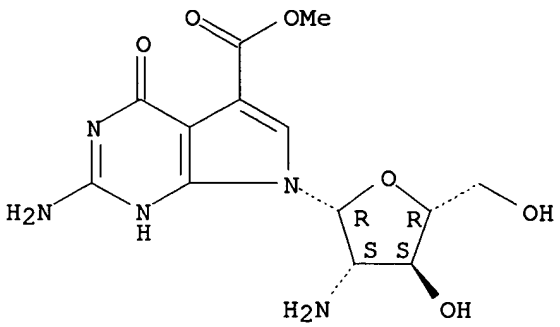
AB Antibiotic AB-116 (I) [**86330-89-4**] was produced by fermentation with Actinoplanes kanagawaensis 232-4 followed by chromatog. Thus, precultured A. kanagawaensis 232-4 (Bikoken 6094, FERM P-6094) was cultured on 100 L broth containing glucose 1.5, soybean powder 1.5, NaCl 0.3, and CaCO3 0.1% for 120 h at 30° under 50 L/min aeration. The broth filtrate was chromatographed over Diaion Hp-20, Amberlite IRC-50 (H type), Sephadex G-10, and Sephadex LH20 to give 500 mg I. UV and IR spectra of I are shown. I inhibited gram-neg. bacteria.

IT **84873-16-5**
RL: BIOL (Biological study)
(from Actinoplanes kanagawaensis)

RN 84873-16-5 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-amino-2-deoxy-β-D-arabinofuranosyl)-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 50 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:125711 CAPLUS

DOCUMENT NUMBER: 98:125711

TITLE: Kanagawamicin, a new aminonucleoside analog antibiotic from Actinoplanes kanagawaensis

AUTHOR(S): Naruto, Shunsuke; Uno, Hitoshi; Tanaka, Akira; Kotani, Hirotada; Takase, Yoshiyuki

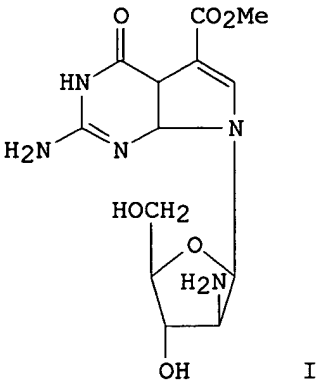
CORPORATE SOURCE: Res. Lab., Dainippon Pharm. Co., Ltd., Suita, 564, Japan

SOURCE: Heterocycles (1983), 20(1), 27-32
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

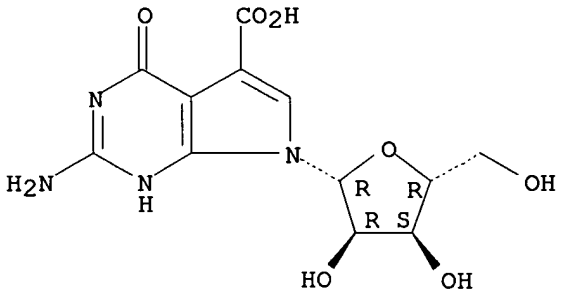
AB The structure of kanagawamicin (I), a new aminonucleoside from Actinoplanes kanagawaensis, was deduced from physicochem. data obtained using the natural compound and its acetates.

IT **81645-08-1**
RL: PRP (Properties)
(NMR spectra of)

RN 81645-08-1 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

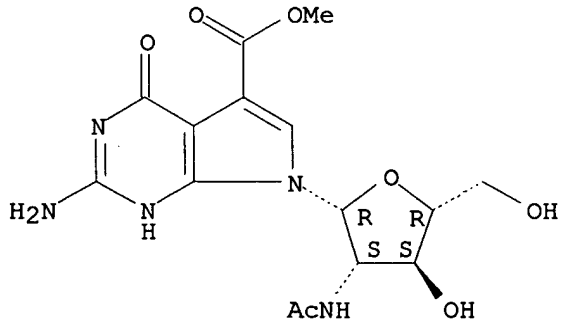


IT **84873-19-8P 84933-22-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 84873-19-8 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-[2-(acetylamino)-2-deoxy-β-D-arabinofuranosyl]-2-amino-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

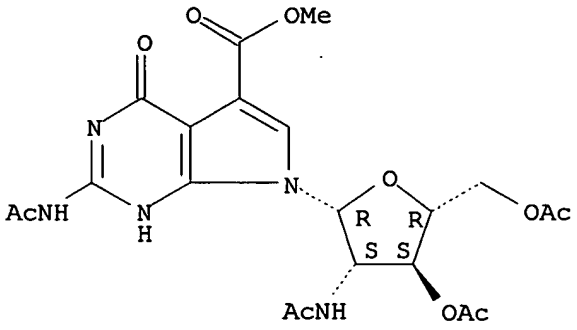
Absolute stereochemistry.



RN 84933-22-2 CAPLUS

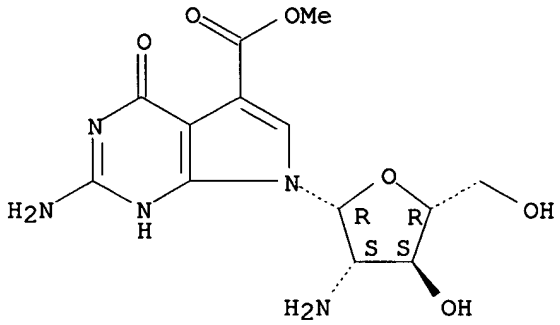
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-(acetylamino)-7-[3,5-di-O-acetyl-2-(acetylamino)-2-deoxy-β-D-arabinofuranosyl]-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

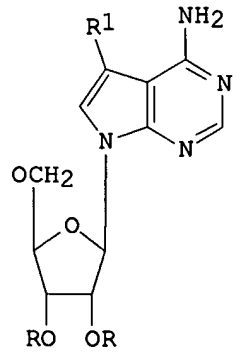


IT **84873-16-5**
RL: PROC (Process)
(structural elucidation of)
RN 84873-16-5 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-7-(2-amino-2-deoxy-β-D-arabinofuranosyl)-4,7-dihydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 51 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:72659 CAPLUS
DOCUMENT NUMBER: 98:72659
TITLE: Nucleosides and nucleotides. 41. Thiocyanation of tubercidin and its derivation to 6-propyl- and 6-cyano derivatives
AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Nucleosides & Nucleotides (1982), 1(2), 191-203
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

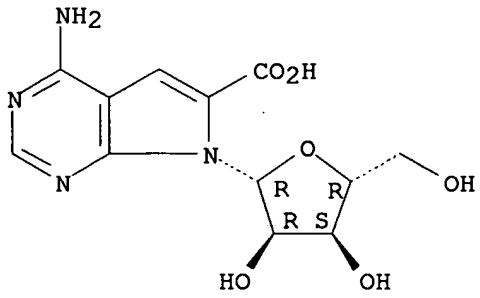
AB Acetylating tubeycidin (I; R = R1 = H) with Ac2O-pyridine gave I (R = Ac, R1 = H), which on thiocyanation with KSCN and Cl gave I (R = Ac, R1 = thiocyanato) (II). II was converted into I (R = Ac, R1 = MeS), I (R = H, R1 = MeSO2) (III) and 6-propyltubercidin. III was converted into 6-cyanotubercidin. Also prepared were 6,5'-O-cyclotubercidins.

IT **77049-87-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77049-87-7 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 52 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:11156 CAPLUS

DOCUMENT NUMBER: 98:11156

TITLE: Pyrrolopyrimidine lethality in relation to ribonucleic acid synthesis in Sarcoma 180 cells in vitro

AUTHOR(S): Ritch, Paul S.; Helmsworth, Marilyn

CORPORATE SOURCE: Dep. Med., Med. Coll. Wisconsin, Milwaukee, WI, 53226, USA

SOURCE: Biochemical Pharmacology (1982), 31(16), 2686-8
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

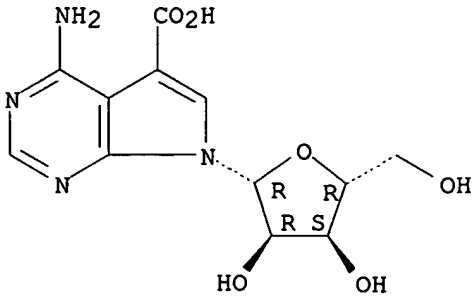
AB Following 1 h exposure of sarcoma 180 cells to sangivamycin (I) [18417-89-5], sangivamycin-amidoxime (II) [22242-94-0], and sangivamycin-amidine (III) [**18418-00-3**] (all 5 + 10-6M), comparable degrees of cell killing were produced. Relatively few cells were killed following exposure to thiosangivamycin (IV) [22242-90-6]. The relative cytotoxicities were I > II > IV, but for RNA synthesis inhibition by the drugs, the order of potency was reversed. At 1 h following exposure to I, IV, and II, total RNA synthesis was inhibited 24, 73, and 57%, resp. Neither adenosine [58-61-7] nor 2'-deoxycoformycin [53910-25-1] (5 + 10-6M) sep. had any effect on cell survival in response to I, but in combination, they protected against the cytotoxic effects of I.

IT **18418-00-3**
RL: PRP (Properties)
(cytotoxicity of, RNA formation inhibition in)

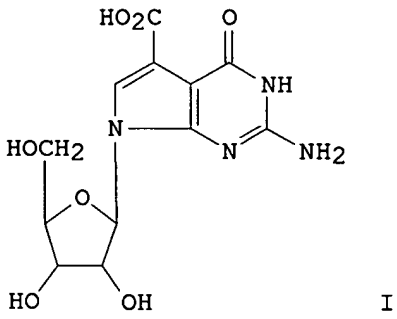
RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 53 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:404557 CAPLUS
DOCUMENT NUMBER: 97:4557
TITLE: Cadeguomycin, a novel nucleoside analog antibiotic. I. The producing organism, production and isolation of cadeguomycin
AUTHOR(S): Tanaka, Nobuo; Wu, Rong Tsun; Okabe, Takayoshi; Yamashita, Hide; Shimazu, Akira; Nishimura, Toshio
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Journal of Antibiotics (1982), 35(3), 272-8
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



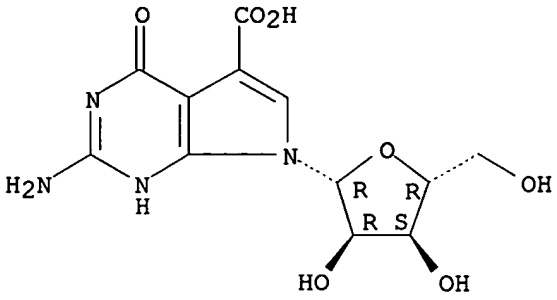
I

AB An actinomycete strain IM7912T was found to produce cadeguomycin (I) [**81645-08-1**], a new nucleoside analog antibiotic, together with tubercidin [69-33-0]. Morphol., cultural and physiol. studies showed that the organism belongs to the species Streptomyces hygroscopicus. Comparison with S. hygroscopicus ISP 5578 revealed that both strains possess similar characteristics except for production of yellow or brownish yellow soluble pigment in some media. I was isolated from the culture filtrate, separated from tubercidin, and purified.

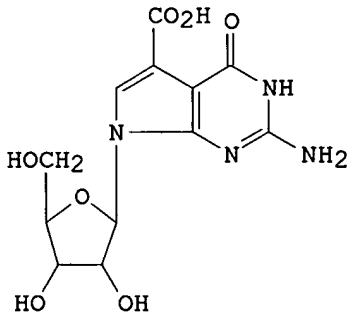
IT **81645-08-1**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(tumor inhibitor, from Streptomyces hygroscopicus)

RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 54 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:196238 CAPLUS
DOCUMENT NUMBER: 96:196238
TITLE: Cadeguomycin, a novel nucleoside analog antibiotic. II. Improved purification, physicochemical properties and structure assignment
AUTHOR(S): Wu, Rong Tsun; Okabe, Takayoshi; Namikoshi, Michio; Okuda, Shigenobu; Nishimura, Toshio; Tanaka, Nobuo
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Journal of Antibiotics (1982), 35(3), 279-84
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



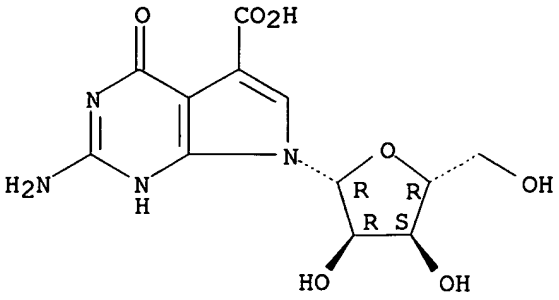
I

AB cadeguomycin (I) [**81645-08-1**] was isolated from the culture filtrate of Streptomyces hygroscopicus by column chromatog. on Amberlite XAD-8 or Amberlite IRA-400, followed by recycling preparative high-pressure column chromatog. The purified antibiotic had a mol. formula of C12H14O7N4 and a m.p. of 231-9°. The structure of I was determined by NMR spectroscopic anal. as 7-carboxy-7-deazaguanosine.

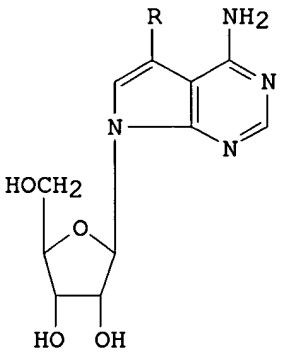
IT **81645-08-1**
RL: BIOL (Biological study)
(antibiotic, from Streptomyces hygroscopicus)

RN 81645-08-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 2-amino-4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 55 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:175411 CAPLUS
DOCUMENT NUMBER: 94:175411
TITLE: Introduction of substituents to the 7(8)-position of 7-deazaadenosine (tubercidin): conversion to toyocamycin
AUTHOR(S): Watanabe, Shinichi; Ueda, Tohru
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Nucleic Acids Symposium Series (1980), 8, s21-s24
CODEN: NACSD8; ISSN: 0261-3166
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

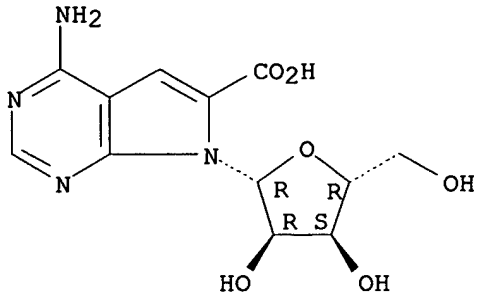


I, R=H
II, R=cyano

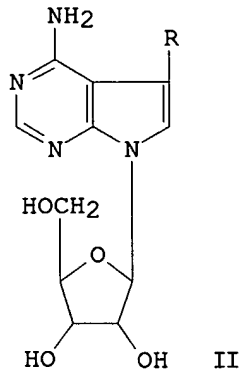
AB Treatment of 2',3',5'-tri-O-acetyl-7-deazaadenosine with ClSCN gave the 7-thiocyanato derivative, which was converted to 7-methylthio and 7-methylsulfone derivs. The thio-Claisen rearrangement and desulfurization of 7-allylthio derivative gave 8-propyl-7-deazaadenosine. The 7-methylsulfone derivative gave the 8-cyano compound by treatment with NaCN. Nitration of triacetylturercidin gave a mixture of the 7- and 8-nitro derivs. The Mannich reaction of tubercidin (I) gave the 7-morpholinomethyl derivative which was converted to the Me, formyl, hydroxymethyl, or cyano derivs. in good yield. The conversion of I to toyocamycin (II) was thus accomplished. Some phys. (spectral and conformational) and biol. (tuberculostatic) properties of these substituted tubercidins are presented.

IT **77049-87-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77049-87-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 56 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:157180 CAPLUS
DOCUMENT NUMBER: 94:157180
TITLE: Pyrrolo[2,3-d]pyrimidine nucleoside antibiotic analogs. Synthesis via organopalladium intermediates derived from 5-mercuritubercidin
AUTHOR(S): Bergstrom, Donald E.; Brattesani, Alan J.; Ogawa, Mark K.; Schweickert, Michael J.
CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA
SOURCE: Journal of Organic Chemistry (1981), 46(7), 1423-31
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



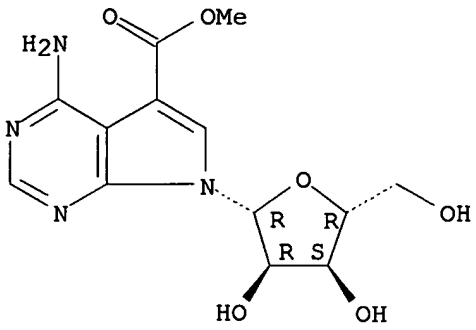
II

AB C-5-substituted pyrrolo[2,3-d]pyrimidine nucleosides were synthesized via reactions of 5-mercuritubercidin (I). Pd-catalyzed carbonylation of I in MeOH gave nucleoside II (R = CO2Me), which was converted to sangivamycin by reaction with NH3. Vinyl analogs (II, R = CH:CHCONH2, CH:CHCN) of sangivamycin and toyocamycin were obtained by a Heck organopalladium olefin coupling reaction. II (R = CH:CHCO2Me), obtained from I and CH2:CHCO2Me in the presence of Li2PdCl4, was converted to (E)-5-(2-bromoethenyl)tubercidin by hydrolysis with base followed by treatment with bromosuccinimide in DMF. The coupling reactions with ethylene, 3-chloro-1-butene, and styrene were also investigated. Ethylene, I and 0.1 M Li2PdCl4 in MeOH lead to II (R = CHMeOMe) and in water to tubercidin (II, R = H), and II (R = CHMeOH). Tubercidin resulted from acid-catalyzed retro-aldol fragmentation. Iodination of I gave II (R = iodo).

IT **18440-68-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ammonia)

RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



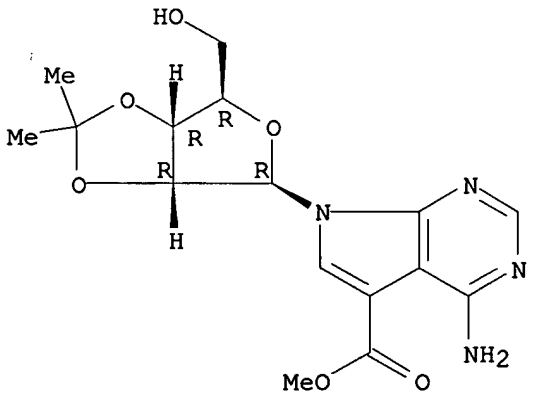
L3 ANSWER 57 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:10332 CAPLUS
DOCUMENT NUMBER: 80:10332
TITLE: 5-Hydroxymethyltubercidin. Synthesis, biological activity, and role in pyrrolopyrimidine biosynthesis
AUTHOR(S): Uematsu, Takayoshi; Suhadolnik, Robert J.
CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Tokyo, Japan
SOURCE: Journal of Medicinal Chemistry (1973), 16(12), 1405
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 5-Hydroxymethyltubercidin (I) [49558-38-5] gave 50% growth inhibition of leukemia L-1210 cells at 4 .tim. 10-7 M while toyocamycin (II) [606-58-6] gave 50% inhibition at 4 .tim. 10-8 M. II inhibits both L-1210 and bacterial (Escherichia coli and Mycobacterium phlei) cells while I is selective, only inhibiting L-1210 cells. When I labeled with 3H was added to cultures of Streptomyces rimosus at the time of II production, there was an uptake of I but no conversion to II. I was prepared from tubercidin-5-carboxylic acid (III) [**18418-00-3**] [prepared from sangivamycin (IV) [18417-89-5]] by conversion to the methyl ester (V), then to the 2',3'-O-isopropylidene derivative and LiAlH4 reduction (method A) or by first protecting the 6-amino group of V with Ph3CCl (method B).

IT **50919-50-1P 50919-51-2P 50919-52-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

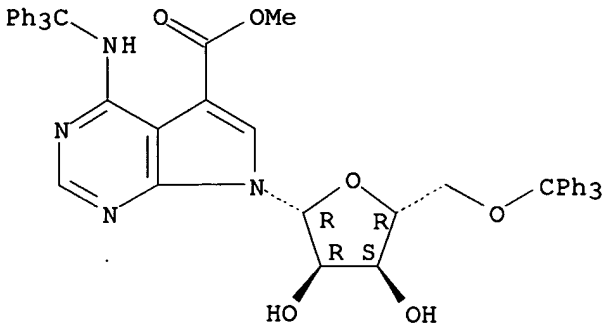
RN 50919-50-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



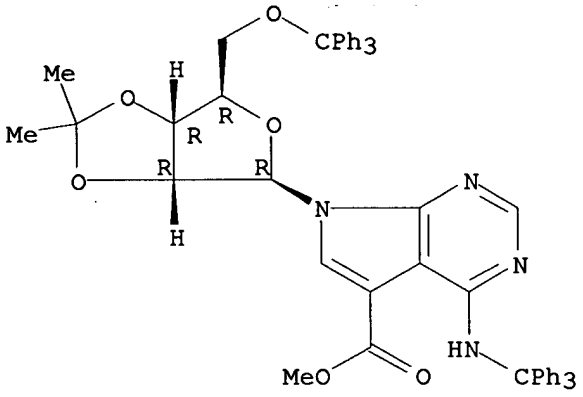
RN 50919-51-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-[(triphenylmethyl)amino]-7-[5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



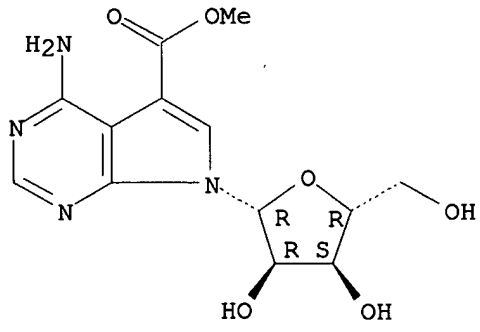
RN 50919-52-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 7-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-4-[(triphenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **18440-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethoxypropane)
RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



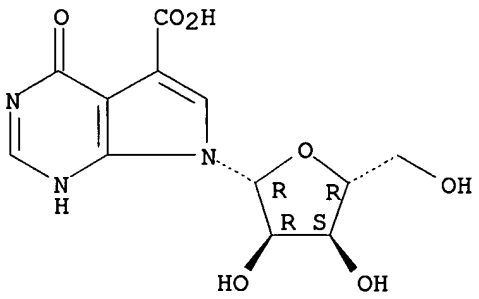
L3 ANSWER 58 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:117587 CAPLUS
DOCUMENT NUMBER: 72:117587
TITLE: Nucleoside antibiotics. VI. Biosynthesis of the pyrrolopyrimidine nucleoside antibiotic toyocamycin by Streptomyces rimosus

AUTHOR(S): Uematsu, T.; Suhadolnik, R. J.
CORPORATE SOURCE: Dep. of Bioorg. Chem., Albert Einstein Med. Center, Philadelphia, PA, USA
SOURCE: Biochemistry (1970), 9(5), 1260-6
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The biosynthesis of the pyrrolopyrimidine nucleoside antibiotic, toyocamycin, elaborated by S. rimosus, has been studied. Adenine-2-14C, but not adenidine-8-14C, is incorporated into toyocamycin. All of the 14C in the toyocamycin from the adenine-2-14C expts. resides in C-2 of toyocamycin. This was shown by the conversion of toyocamycin into the 3-carboxyethyl derivative C-2 of toyocamycin was released as formic acid by heating 5-carboxamido-3-(2-carboxyethyl)-4-hydro-xy-7β-D-ribofuranosylpyrrolo[2,3-d]pyrimidine (I) in alkali. 5-Carboxy-4-hydroxy-7-(β-D-ribofuranosyl)pyrrolo[2,3 - d]pyrimidine (II), synthesized from the intermediate 2-amino-4-carboxy-3-carbonyl - [N-(2-carboxyethyl)]-1-β-D-ribofuranosylpyrrole by treatment with formic acid and Ac2O, was not radioactive. Sangivamycin, 5-carboxamido-4-hydroxy-7-(β-D - ribofuranosyl)pyrro-lo[2,3-d]pyrimidine (III), 4-hydroxypyrrolo[2,3-d]pyrimidine, I, and II were all isolated and crystallized, and their structures were rigorously characterized. The isolation of formic acid from I was unequivocally established. These data provide evidence that N-7 and C-8 of the imidazole ring of a purine are lost during the biosynthesis of the pyrrole ring of toyocamycin. III has been alkylated in good yields with β-propiolactone at N-3 of the pyrrolopyrimidine ring to form the carboxyethyl nucleoside I. This procedure affords an excellent method for opening of the pyrimidine ring and the isolation of C-2 as formic acid. The studies reported here add another role of purines in the biosynthesis of naturally occurring compds.

IT **28070-52-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28070-52-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 59 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:413308 CAPLUS
DOCUMENT NUMBER: 71:13308
TITLE: Pyrrolopyrimidine nucleosides. III. Total synthesis of toyocamycin, sangivamycin, tubercidin, and related derivatives
AUTHOR(S): Tolman, Richard L.; Robins, Roland K.; Townsend, Leroy B.
CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA
SOURCE: Journal of the American Chemical Society (1969), 91(8), 2102-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 71:13308
GI For diagram(s), see printed CA Issue.

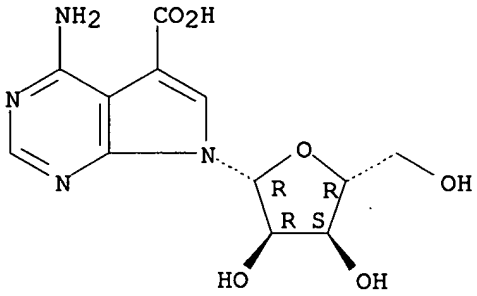
AB The structure of toyocamycin and sangivamycin were unequivocally established as 4-amino-5-cyano-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (I) and 4-amino-5-carboxamido-7-(β-D-ribofuranosyl)pyrrolo-[2,3-d]pyrimidine (II), resp. The total synthesis of all the presently known pyrrolo[2,3-d]pyrimidine nucleoside antibiotics (toyocamycin, sangivamycin, and tubercidin) has now been accompanied via the acid-catalyzed fusion procedure. The synthesis of several new pyrrolo[2,3-d]pyrimidine derivs. required for utilization in the fusion procedure is reported. Factors which are involved in a successful fusion reaction, e.g., the number and magnitude of electron-withdrawing substituents and the juxtaposition of these substituents in relation to the site of glycosidation, are discussed.

IT **18418-00-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 60 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:86268 CAPLUS

DOCUMENT NUMBER: 70:86268

TITLE: Sangivamycin and derivatives

INVENTOR(S): Rao, Koppaka V.; Marsh, William S.; Renn, Donald W.

PATENT ASSIGNEE(S): Pfizer, Chas., and Co., Inc.

SOURCE: U.S., 10 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3423398	A	19690121	US 1965-454637	19650510

PRIORITY APPLN. INFO.: US 1965-454637 A 19650510

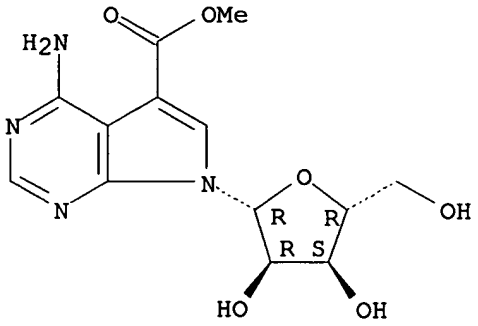
AB Fermentation by a strain of Streptomyces rimosus produces sangivamycin (I), 4-amino-5-carboxamido-7-(D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine, and N-(lower alkyl) substituted amides, a deamidohydrazido derivative, N-oxide, monohydrate, and salts. All are active against tumors. Thus, a slant of S. rimosus ATCC 14673 was incubated for 48 hrs. at 28° in a medium of glucose 10, soy bean meal 15, distillers' solubles 2.5, K2HPO4 2, NaCl 1, and CaCO3 0.5 g./l. and propagated in the same medium with air at 1 volume/volume/min. for 72 hrs. The filtered broth was highly active against HeLa cells in tissue culture. Adsorbing on C at pH 4, eluting with 0.05N HCl in MeOH, dissolving the neutralized and dried eluate in MeOH, and passing through DEAE-cellulose gave an effluent from which I was again adsorbed, eluted, and finally crystallized from aqueous pyridine as I.H2O in rectangular prisms, m. 258-60°. The reineckate, m. 170°, also had a high inhibitory activity against tumors. Heating 2 g. I in 200 cc. 2N NaOH gave the deamido derivative of I, m. 236-8°, C12H14O6N4.HCl, its Me ester m. 216-8°, and its hydrazide 238-40°. Refluxing 0.2 g. tetraacetyl-I in 25 cc. CHCl3 with 0.3

cc. POCl3, concentrating, diluting with H2O and extracting the neutralized solution with CHCl3 gave tetraacetyltoyocamycin, which was separated as the picrate, m. 160-2°. Treating I in AcOH with H2O2 gave the N-oxide, m. 276-8°.

IT **18440-68-1 21090-38-0**
RL: BIOL (Biological study)
(neoplasm inhibitors)

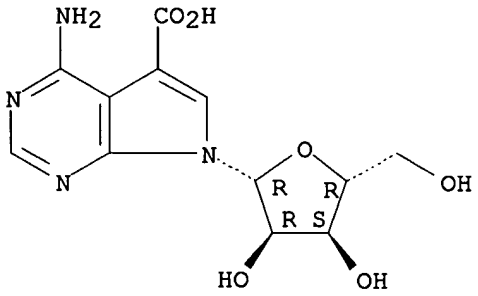
RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 21090-38-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

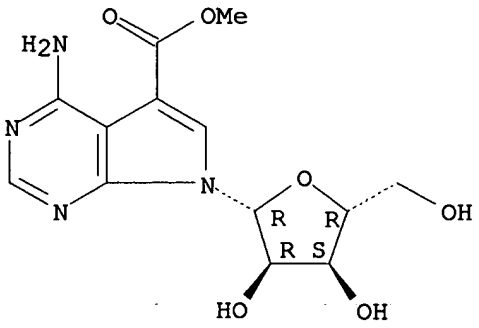
L3 ANSWER 61 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:497071 CAPLUS
DOCUMENT NUMBER: 69:97071
TITLE: Structure of sangivamycin
AUTHOR(S): Rao, Koppaka V.
CORPORATE SOURCE: John L. Smith Mem. for Cancer Res., Chas. Pfizer and Co., Inc., Maywood, NJ, USA
SOURCE: Journal of Medicinal Chemistry (1968), 11(5), 939-41
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Sangivamycin (I) is an antitumor substance, a metabolite of a streptomycete culture, and shows spectral properties similar to those of nucleosides. The presence of a pentose residue was established indirectly by periodate oxidation and hydrolysis. The compound also has an aromatic amino group and a carboxamide group. Some of the similarities in properties to toyocamycin (II) led to the hypothesis that sangivamycin may be closely related to this compound This hypothesis is shown to be correct in that

sangivamycin has a carboxamide group and toyocamycin has a nitrile group on the same carbon skeleton. This relationship is established by three different methods. A brief study of the biological activity of some of the derivs. of sangivamycin is described.

IT **18440-68-1P 21090-38-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

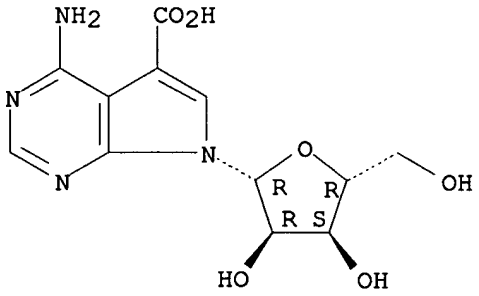
RN 18440-68-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 21090-38-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L3 ANSWER 62 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:78540 CAPLUS
DOCUMENT NUMBER: 68:78540
TITLE: Pyrrolo[2,3-d]pyrimidine nucleoside antibiotics. Total synthesis and structure of toyocamycin, unamycin B, vengicide, antibiotic E-212, and sangivamycin (BA-90912)
AUTHOR(S): Tolman, Richard L.; Robins, Roland K.; Townsend, Leroy B.
CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA
SOURCE: Journal of the American Chemical Society (1968), 90(2), 524-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 68:78540
GI For diagram(s), see printed CA Issue.
AB A total synthesis of toyocamycin (I, R = CN, R1 = H, R2 = NH2, R3 = H) (II) and sangivamycin (I, R = CONH2, R1 = H, R2 = NH2, R3 = H) (III) and

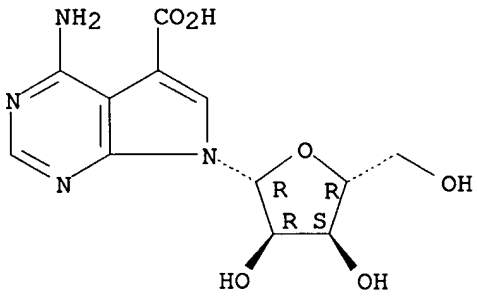
the unequivocal assignment of their structures are reported. Ring closure of 2-amino-5-bromo-3,4-dicyanopyrrole with formamidine acetate in EtOCH2CH2OH at reflux temperature gave 4-amino-6-bromo-5-cyanopyrrolo[2,3-d]pyrimidine (IV, R2 = NH2) (IVb). IVb, Ac2O, and xylene refluxed 18 hrs. gave the monoacetylated derivative (IV, R2 = NHCOMe) (IVc). IVc and tetra-O-acetyl-β-D-ribofuranose heated at 175° in the presence of bis(p-nitrophenyl) phosphate 25 min. followed by column and preparative layer chromatog. gave the acetylated nucleoside (I, R = CN, R1 = Br, R2 = NHCOMe, R3 = Ac) (V). Treatment of V with methanolic NH3 at room temperature resulted in complete deacetylation to 4-amino-6-bromo-5-cyano-7-(β-D-ribofuranosyl)pyrrolo[2,3-d]pyrimidine (I, R = CN, R1 = Br, R2 = NH2, R3 = H) (VI), which was debrominated over 5% Pd-C with H to give II. A rigorous comparison of authentic samples of unamycin B, antibiotic E-212, and vengicide proved that these antibiotics are identical with II. Treatment of VI with 30% H2O2 in concentrated NH4OH at room temperature gave the corresponding 5-carboxamido derivative (I, R = CONH2, R1 = Br, R2 = NH2, R3 = H), which on debromination gave III. Addnl. evidence for the structural assignment of II and III was furnished by the conversion of sangivamycic acid to the related pyrrolo[2,3-d]pyrimidine antibiotic tubercidin (I, R = R1 = R3 = H, R2 = NH2).

IT **18418-00-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18418-00-3 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-amino-7-β-D-ribofuranosyl- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



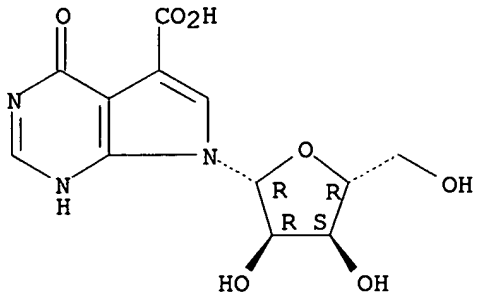
L3 ANSWER 63 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1965:441749 CAPLUS
DOCUMENT NUMBER: 63:41749
ORIGINAL REFERENCE NO.: 63:7524e-f
TITLE: Antitumor activities and structural relation of tubercidin, toyocamycin, and their derivatives
AUTHOR(S): Saneyoshi, Mineo; Toluzen, Reiko; Fukuoka, Fumiko
CORPORATE SOURCE: Natl. Cancer Center Res. Inst., Tokyo
SOURCE: Gann (1965), 56(2), 219-22
CODEN: GANNA2; ISSN: 0016-450X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Normal young adults of Swiss mice and Nakahara-Fukuoka sarcoma (N-F) were used. Among the compds. related to toyocamycin, the active cancericidal action in vitro depended on the coexistence of an amino group in the mol. at the 4 position, CN at the 5 position, and ribofuranose at the 7 position. When the 4 position is deaminated with HNO2 (deaminohydroxytoyocamycin) the activity is markedly diminished with simultaneous decrease of toxicity. Tubercidin, is less toxic and less cancericidal than toyocamycin, and the in vitro cancericidal action is not shared by its hydroxyl derivative, deaminohydroxytubercidin. In in vivo tests, tubercidin as well as deaminohydroxytubercidin showed a slight tumor-inhibiting effect, while 4-aminopyrrolo[2,3-d]pyrimidine and 4-hydroxypyrrolo[2,3-d]pyrimidine, which are aglycons of tubercidin and deaminohydroxytubercidin, resp., are both without antitumor action and have a very low toxicity.

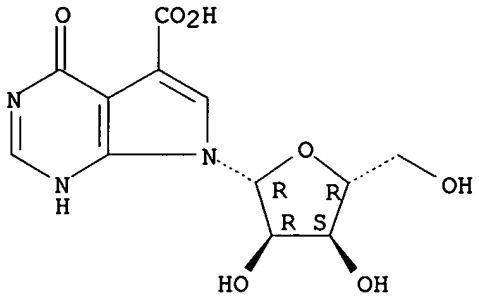
IT **28070-52-2**, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-
(as neoplasm inhibitor)
RN 28070-52-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 64 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:441748 CAPLUS
DOCUMENT NUMBER: 63:41748
ORIGINAL REFERENCE NO.: 63:7524b-e
TITLE: Pharmacological research on new acetylenic derivatives with hypotensive action
AUTHOR(S): Cascio, G.; Fabra, I.; Madonia, P.; Mantia, G.; Sprio, V.
CORPORATE SOURCE: Univ. Palermo, Italy
SOURCE: Farmaco, Edizione Scientifica (1965), 20(5), 336-50
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
AB The synthesis and pharmacol. activity of phenylacetylene derivs. are described. EtMgBr is added dropwise to an ether solution of phenylacetylene and the mixture is heated on a water bath for 1 hr., cooled, and an ether solution of acetophenone is added slowly with vigorous stirring. After 12 hrs., the solution is heated on a water bath for 2 hrs. The ether phase is separated after acidification with H2SO4 to give 2,4-diphenyl-3-butyn-2-ol-1-al oxime (I) white needles, m.p. 138-40° (benzene). Similarly, 5-phenyl-3-methyl-4-pentyn-3-ol-2-one oxime (II) is prepared from isonitrosomethyl ethyl ketone as white prisms, m.p. 79° (benzene + petroleum ether). The L.D·50 in the mouse is 1.250 g. I/kg., intraperitoneally, and in the rat 8.750 g./kg., orally. Corresponding values for II are 1.750 g./kg., and 3.125 g./kg., resp. In doses between 100 and 200 mg./kg., I and II show no effect on the central nervous system. I is somewhat oil soluble and shows a slight hypotensive activity. II is very soluble in oil and shows a strong and quick hypotensive effect when administrated either intraparenterally or orally. By 120 min. after oral administration of 100 mg. II/kg., the arterial pressure is decreased. This decrease continues for some hrs., and then the hypotensive activity is exhausted very slowly. When the dose is 10% as large, the hypotensive activity is obtained only by a prolonged treatment. In hypotensive doses II does not modify the diuresis. II shows no ganglioplegic, sympathicolytic or parasympathicomimetic effect. By 2 hrs. after administration of a single high dose, the catechol amine levels are decreased in the blood and cerebral tissue, whereas they increase in adrenal tissue. At the end of the hypotensive effect, the catechol amine levels in blood and in brain are higher than normal, whereas in adrenal tissue they are decreased.
IT **28070-52-2**, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-
(as neoplasm inhibitor)
RN 28070-52-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4,7-dihydro-4-oxo-7-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 65 OF 65 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:27298 CAPLUS
DOCUMENT NUMBER: 58:27298
ORIGINAL REFERENCE NO.: 58:4557g-h,4558a-e
TITLE: Chemical structure of toyocamycin
AUTHOR(S): Okuma, Kazuhiko
CORPORATE SOURCE: Inst. Phys. Chem. Res., Tokyo
SOURCE: J. Antibiotics (Tokyo) Ser. A (1961), 14, 343-52
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 55, 27330f. Streptomyces Number 1922 was cultured in a medium containing soluble starch 1.5, glucose 0.5, Polypeptone 0.5, meat extract 0.5, NaCl 0.5, K2HPO4 0.01, and soybean meal 1.0% (pH 7.0) and toyocamycin (I) was isolated from broth filtrate by adsorption on C-1 resin (salicylic acid type), elution with 80% aqueous Me2CO, concentration in vacuo, extraction with BuOH at pH 7.0, back-extraction with 0.5N HCl, and concentration in vacuo. I, C12H13N5O4 (EtOH) or C12H13N5O4.H2O (H2O), was colorless needles, m. 237° (decomposition) (EtOH), [α]16D -45.7° (c 1.05, 0.1N HCl). I gave pos. periodate, and neg. Fehling, biuret, Pauly, FeCl3, and ninhydrin tests, was soluble in AcOH and acid, moderately soluble in MeOH, EtOH, Me2CO, dioxane, and BuOH, sparingly soluble in H2O and Et2O, and insol. in petr. ether, EtOAc, and CHCl3. I formed a monopicrate, decomposed 225-6° (H2O). I with Ac2O in C5H5N yielded a tetra-Ac derivative, m. 100°. I, heated at 70° with NaNO2 in glacial AcOH, yielded a deaminohydroxy derivative of I (II), C12H12N4O5, m. 262-3°, λ 264 mμ (ε 13,870, 0.1N HCl) and 228 and 274.5 mμ (ε 12,176 and 15,330, resp., 0.1N NaOH). I consumed 1 mole of periodate without formation of HCO2H. II absorbed H on Pd-C in N HCl to yield a deaminohydroxy-decyanoaminomethyl derivative of I (III), C12H16N4O5, decomposed 246-8° (H2O), λ 260 mμ (ε 8786, 0.1N HCl), 217 and 271 mμ (ε 18,493 and 9597, resp., 0.1N NaOH), and orange yellow with ninhydrin. I refluxed in 3N HCl for 4 hrs. under N gave needles, which yielded, on deamination with NaNO2 in AcOH, a deaminohydroxydecyanocarboxy derivative of I (IV), C12H15N3O6.2H2O, decomposed 278° (H2O), λ 230 and 274 mμ (ε 12,987 and 11,921, resp., 0.1N HCl), and 230 and 277 mμ (ε 9557 and 13,453, resp., 0.1N NaOH). D-Ribose was found in the hydrolyzate from I and Dowex-50 (H). II, heated at 150° in a sealed tube with HI and red P for 5 hrs., yielded 4-hydroxypyrrolo[2,3-d]pyrimidine (V), on precipitation with AgNO3, removal of Ag, and sublimation in vacuo. V, C6H5N3O, decomposed 336-40°, λ 263 mμ (ε 9650, 0.1N HCl) and 265 mμ (ε 10,300, 0.1N NaOH). V was also obtained by alkali fusion of I at 250-60° 30 min., absorption on C-1 ion exchange resin (H), elution with 80% aqueous Me2CO, chromatography on cellulose powder with BuOH-MeOH-H2O (2:1:2), concentration in vacuo, and sublimation. III was heated at 150° for 4 hrs. in a sealed tube with HI and red P, the mixture concentrated in vacuo, the insolubles in cold NH4OH warmed for 10 min. in HCl, and the filtrate was dried to 4-hydroxy-5-aminomethylpyrrolo[2,3-d]pyrimidine-HCl (VI) (decomposed above 300°), which was purified as the helianthate, C21H23N7SO4, decomposed 248-50° (H2O). 4-Hydroxy-5-[bis(ethylthio)methyl]pyrrolo[2,3-d] pyrimidine (VII) was isolated by

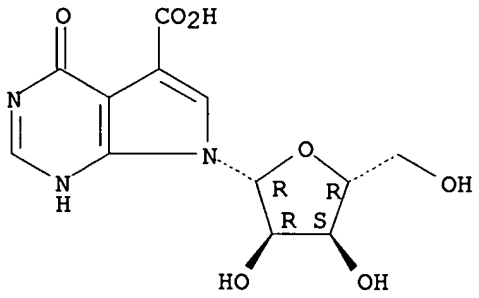
refluxing VI in AcOH and hexamethylenetetramine 10 min., adsorbing on and eluting from C-1 ion exchange resin (H), concentrating in vacuo, and chromatographing on cellulose powder, C11H15N3S2O, decomposed 230-3°, λ 272 mμ (ε 9188, EtOH). 4-Hydroxy-5-methylpyrrolo[2,3-d]pyrimidine (VIII) was isolated by refluxing VII in 80% aqueous EtOH with Raney Ni, concentrating in vacuo, and subliming in vacuo, C7H7N3O, decomposed 280-2°, λ 225 and 273 mμ (ε 9663 and 7250, 0.1N HCl), and 271 mμ (ε 9020, 0.1N NaOH). VIII was identical with that synthesized from Et cyanoacetate via α-bromopropionaldehyde diethyl acetal, Et (α-cyano-β-methyl-γ,γ-diethoxy)butyrate, 2-mercapto-4-hydroxy-5-(1-methyl-2,2-diethoxy)-ethyl-6-aminopyrimidine, and 4-hydroxy-6-(1-methyl-2,2-diethoxy)ethyl-6-aminopyrimidine (Brit. 812,366, CA 54, 592i; Davoll, CA 54, 8840d). Thus, I [R = (D-ribofuranosyl)] was proposed as the structure of toyocamycin.

IT **89305-63-5**, 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-, dihydrate
(preparation of)

RN 89305-63-5 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxylic acid, 4-hydroxy-7-β-D-ribofuranosyl-, dihydrate (7CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 H_2O

=>

---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	336.58	503.73

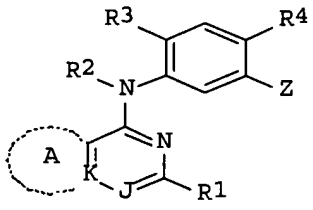
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-48.75	-48.75

STN INTERNATIONAL LOGOFF AT 15:56:12 ON 16 MAY 2006

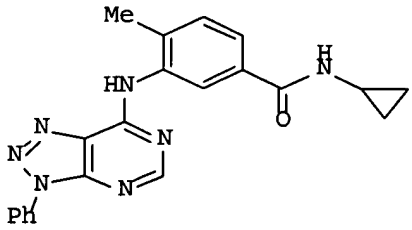
L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:409524 CAPLUS Full-text
DN 142:463438
TI Preparation of phenylamine substituted bicyclic heterocyclic compounds useful as kinase inhibitors
IN Das, Jagabandhu; Hynes, John; Leftheris, Katerina; Lin, Shuqun; Wrobleski, Stephen T.; Wu, Hong
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005042537	A1	20050512	WO 2004-US35116	20041022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005143398	A1	20050630	US 2004-970420	20041021
PRAI US 2003-513285P	P	20031022		

OS MARPAT 142:463438
GI



I



II

AB Title compds. I [J = N or CR5; R1 and R5 independently = H, OH, halo, CN, etc.; R2 = H or alkyl; R3 and R4 independently = H, (un)substituted-alkyl, OH, MeO, halo, etc.; K = N or C; Z = NHR6, CONR6R7, NR6CO2R7, etc.; R6 = H or (un)substituted alkyl; R7 = H, OH, alkoxy, etc.; Ring A = fused heterocycle or carbocycle], and their pharmaceutically acceptable salts, prodrugs, and solvates thereof, are prepared and disclosed as kinase inhibitors. Thus, e.g., II was prepared by reaction of 4-chloro-1-phenyl- 1,2,3,5,7-azaindene

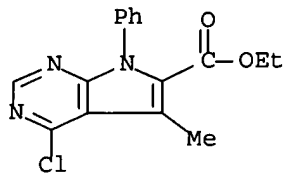
with 3-amino-4-methyl-N-cyclopropylbenzamide. I have shown activity as inhibitors of p38α/β enzymes and TNF-α (no data).

IT **245728-43-2**

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenylamine substituted bicyclic heterocyclic compound as kinase inhibitors)

RN 245728-43-2 CAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-chloro-5-methyl-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:506580 CAPLUS Full-text
DN 139:79178
TI Synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivatives and use as phosphodiesterase VII inhibitors and in combination with other agents
IN Eggenweiler, Hans-Michael; Wolf, Michael
PA Merck Patent GmbH, Germany
SO Ger. Offen., 36 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10163991	A1	20030703	DE 2001-10163991	20011224
	CA 2471538	AA	20030710	CA 2002-2471538	20021108
	WO 2003055882	A1	20030710	WO 2002-EP12533	20021108
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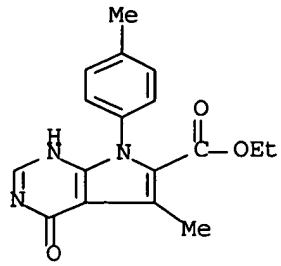
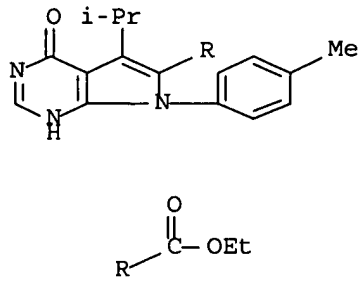
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002367090	A1	20030715	AU 2002-367090	20021108
	EP 1458722	A1	20040922	EP 2002-805744	20021108
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	BR 2002015308	A	20041221	BR 2002-15308	20021108
	CN 1608067	A	20050420	CN 2002-826034	20021108
	JP 2005520801	T2	20050714	JP 2003-556412	20021108
	US 2005059686	A1	20050317	US 2004-500040	20040623
	ZA 2004005859	A	20050517	ZA 2004-5859	20040722
PRAI	DE 2001-10163991	A	20011224		
	WO 2002-EP12533	W	20021108		

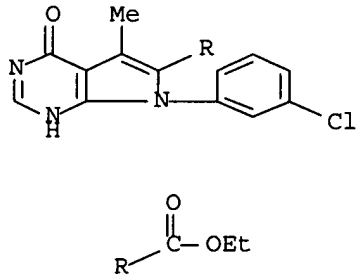
OS MARPAT 139:79178
AB The invention concerns the synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs., their physiol. acceptable salts, stereoisomers, solvates, mixts. thereof and their use as phosphodiesterase VII inhibitors in the treatment of diseases that are influenced by the phosphodiesterase VII regulation of human eosinophil activation and degranulation. Osteoporesis, tumors, cachexia, atherosclerosis, rheumatoid arthritis, multiple sclerosis, diabetes mellitus, AIDS, autoimmune and heart diseases can be treated with the drugs. Thus the synthesis of 5-isopropyl-4-oxo-7-p-tolyl-4,7-dihydro- 3H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid Et ester and analog compds. is described along with injection, suppository, tablet and other formulations.
IT **120049-86-7P 552298-54-1P 552298-55-2P**
552298-56-3P 552298-57-4P 552298-58-5P
552298-59-6P 552298-60-9P 552298-61-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 3H-pyrrolo[2,3-d]pyrimidine derivs. and use as phosphodiesterase VII inhibitors and in combination with other agents)
RN 120049-86-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-7-(4-methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



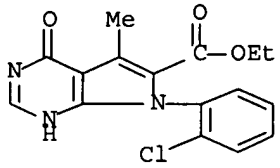
RN 552298-54-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-(1-methylethyl)-7-(4-methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



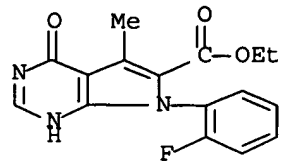
RN 552298-55-2 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(3-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



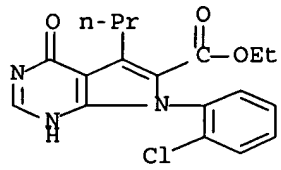
RN 552298-56-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



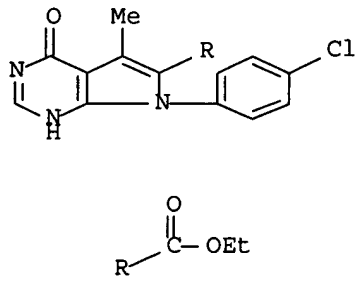
RN 552298-57-4 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-fluorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



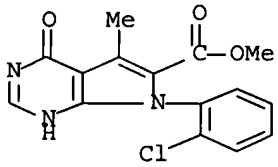
RN 552298-58-5 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-4-oxo-5-propyl-, ethyl ester (9CI) (CA INDEX NAME)



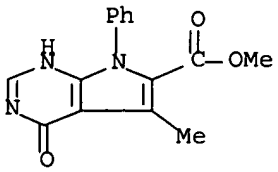
RN 552298-59-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(4-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



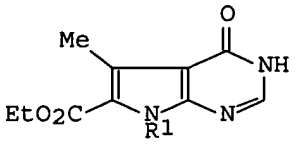
RN 552298-60-9 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-(2-chlorophenyl)-4,7-dihydro-5-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 552298-61-0 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1989:173185 CAPLUS Full-text
DN 110:173185
TI Reactions with heterocyclic enaminonitriles. Synthesis of pyrrolo[2,3-b]pyridine, pyrrolo[2,3-d]pyrimidine and pyrrole derivatives
AU Abdelhamid, Abdou O.; Abdel-Galil, Fathy M.; Saleh, Sohair S.
CS Fac. Sci., Cairo Univ., Giza, Egypt
SO Heterocycles (1988), 27(8), 1861-6
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
OS CASREACT 110:173185
GI



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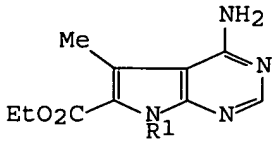

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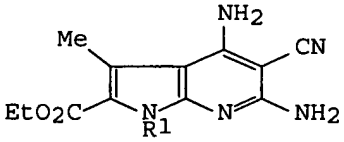

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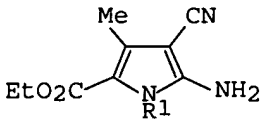
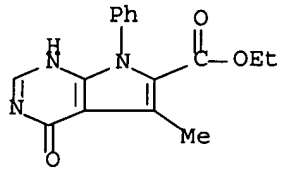
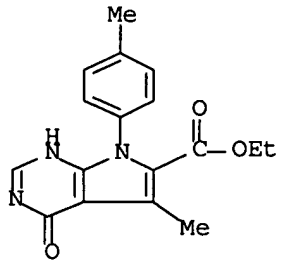


IV

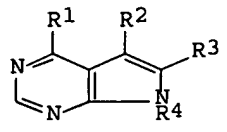
AB Pyrrolopyrimidines I and II and pyrrolopyridines III (R1 = Ph, tolyl) were prepared from aminopyrrolecarbonitriles IV. IV were heated with aqueous HCO2H to give I. The reaction of IV with HCONH2, HCO2H, and DMF gave II. III were prepared from IV and CH2(CN)2; IV and NCCH2CO2Et also gave pyrrolopyridines.
IT **120049-85-6P 120049-86-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 120049-85-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-4-oxo-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 120049-86-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4,7-dihydro-5-methyl-7-(4-methylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

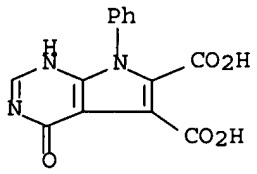


L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1987:43451 CAPLUS Full-text
DN 106:43451
TI Receptor affinity of xanthine oxidase inhibitors: structural requirements. An example of computer-assisted drug design (CADD) and molecular modeling
AU Folkers, Gerd
CS Pharm. Inst., Univ. Tuebingen, Tuebingen, 7400, Fed. Rep. Ger.
SO Deutsche Apotheker Zeitung (1986), 126(41), 2243-7
CODEN: DAZEA2; ISSN: 0011-9857
DT Journal
LA German
GI

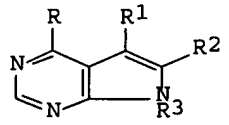


I

AB Structure-activity relations for pyrrolopyrimidines (I; R1 = NH2, OH; R2 = R3 = CO2H, CHO, or Me; R4 = iso-Pr or Ph) as inhibitors of xanthine oxidase (XOD) [9002-17-9] were studied by using computer-assisted drug design and mol. modeling. The inhibition of XOD by I(R1 = NH2; R2 = R3 = CO2H; R4 = Ph) [101153-20-2] and I(R1 = OH; R2 = R3 = CO2H; R4 = Ph [**101153-21-3**]) was substituent dependent. The tautomeric capability of the pyrimidine portion of I was an essential feature for the interaction of I with the enzyme receptor.
IT **101153-21-3**
RL: BIOL (Biological study)
(xanthine oxidase inhibition by, structure in relation to)
RN 101153-21-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5,6-dicarboxylic acid, 4,7-dihydro-4-oxo-7-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:141712 CAPLUS Full-text
DN 104:141712
TI Active site molecular modeling of xanthine oxidase inhibitors with antiinflammatory activity
AU Folkers, Gerd; Hoeltje, Hans Dieter
CS Pharm. Inst., Univ. Berne, Bern, CH-3012, Switz.
SO Journal of Molecular Graphics (1985), 3(4), 146-50
CODEN: JMGRDV; ISSN: 0263-7855
DT Journal
LA English
GI

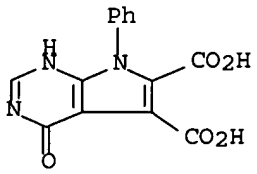


I

AB QSAR in the interaction of antiinflammatory pyrrolopyrimidines (I; R = OH or NH2; R1 and R2 = CO2H, Me, or CHO; R3 = iso-Pr or Ph) with the active site of xanthine oxidase [9002-17-9] were examined with the use of e MO and quantum mol. mech. methods. The results explain the active site preference and decreasing inhibitory potency of the Me, CHO, and CO2H derivs.

IT **101153-21-3**
RL: BIOL (Biological study)
(xanthine oxidase inhibition by, QSAR in)

RN 101153-21-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-5,6-dicarboxylic acid, 4,7-dihydro-4-oxo-7-phenyl- (9CI) (CA INDEX NAME)



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=> d l2; d his; log y
L2 HAS NO ANSWERS
L1              STR
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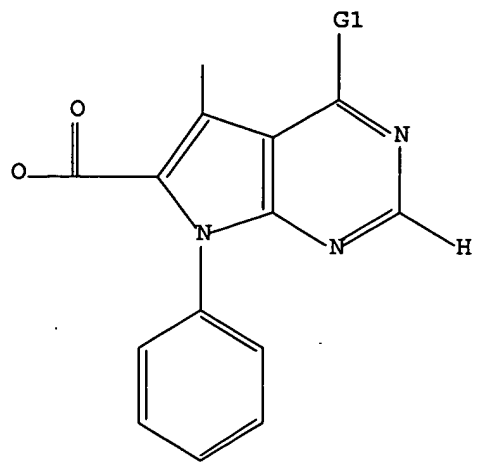


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G1 X,O

Structure attributes must be viewed using STN Express query preparation.
L2              QUE  ABB=ON  PLU=ON  L1

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     FILE 'REGISTRY' ENTERED AT 08:34:16 ON 04 MAY 2006
L1              STRUCTURE UPLOADED
L2              QUE L1
L3            1 S L2
L4           12 S L2 FUL

     FILE 'CAPLUS' ENTERED AT 08:35:32 ON 04 MAY 2006
L5            5 S L4

     FILE 'STNGUIDE' ENTERED AT 08:36:09 ON 04 MAY 2006


COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                0.06     193.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -3.75

STN INTERNATIONAL LOGOFF AT 08:36:16 ON 04 MAY 2006
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